Hall thruster plasma interactions with solar cell arrays on SMART–1

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Abstract

Interactions of ambient plasma with spacecraft are known to cause multiple degenerating effects. Sputtering on surfaces, material deposition, erosion, and electrostatic charging lead to shorter lifetimes and decreased efficiency of technical systems. Due to the increased application of electric propulsion the detailed investigation of the appearing plasma interactions is an issue of highest importance. Differential charging causes potentials of up to several hundred Volt. Malfunction or destruction of sensible electronic devices, short circuits due to sparking, and degradation of solar cells may result in partial or even total fallout of a satellites power system. Hence an accurate and reliable model for the calculation of the expected potentials is of vital importance for the design of future satellites. The plasma and spacecraft environment simulation SmartPIC has been developed for this purpose. Recently an unexplained cyclic variation of the spacecraft floating potential has been observed on the first European Moon mission SMART–1. SmartPIC has been able to qualitatively confirm a correlation with the rotation of the solar arrays. However, detailed review of plasma physics at low densities and high electric fields has shown that the linear Langmuir sheath theory and the quasineutrality assumption underlying the utilized model for the calculation of floating potentials are outranged and inaccurate for the special configuration on SMART–1. This is the motivation for the development of a new kind of electron fluid model capable of the self-consistent calculation of electron and ion densities throughout a large spatial domain. Spadework included the implementation of an advanced multigrid generation technique allowing for high spatial resolution and precise adaption to arbitrary shaped spacecraft surfaces by domain-subdivisioning. A modified multigrid solver algorithm for the Poisson equation guarantees fast and accurate determination of the electric potential that represents the main coupling field in the plasma. The theory of the advanced electron fluid model has been developed, however implementation is still in progress. All new implementations have been tested and verified. Even without fully applying the new fluid model promising results could be obtained. RPA measurements taken on SMART–1 as well as in ground tests have been predicted by SmartPIC at high accuracy. Floating potentials have been calculated by SmartPIC and show very good agreement with the on-board data obtained on SMART–1. A detailed and systematic investigation of the backflow currents has shown that small interconnector structures on the solar arrays biased to high positive potentials play a dominant role in the formation of spacecraft charging. These results will be a valuable input for the design of satellites.
Curriculum Vitae

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Chapter 1

Introduction

1.1 The SMART–1 Mission

SMART–1 is the first mission of ESAs \textit{Small Missions for Advanced Research and Technology} program. This incentive has been started to provide early opportunities for development and test of new technologies essential for future cornerstone missions. SMART–1 is the first European built spacecraft using primary electric propulsion for an interplanetary mission. The demonstration of this new technology has been the main objective of SMART–1. Besides a long list of ambitious tasks and experiments had to be accomplished. Projects in the SMART program always have to be very economical. The financial frame of 100 million € is about one fifth of usual ESA missions. This results in very sophisticated, light weighted spacecraft. SMART–1 weighted only 366.5kg and, in packed state, did not occupy much more than a cubic meter space on the launcher.

In fact, this mission is Europes first attempt to send a spacecraft to the moon. Numerous instruments are packed on board to acquire exact geological and chemical maps of our next neighbor in space. One objective is to eventually find indices of water ice, an essential need for long-term manned lunar missions.

On September 27\textsuperscript{th}, 2003 SMART–1 has been launched together with two communication satellites onboard an Ariane 5 rocket from French Guiana. It has been lifted to a geostationary transfer orbit (GTO) from where it started to accelerate by solely utilizing its Hall thruster ion engine. Due to only 70 mN thrust at nominal conditions the trajectory has been spiral shaped and increased only slowly taking 332 orbits around earth before the spacecraft was captured on November 15\textsuperscript{th}, 2004 by the moons gravity into a lunar orbit. The final position has been reached after 15 months total flight time on January 13\textsuperscript{th}, 2005. Its current orbit ranges from 300 – 3,000 km above the lunar surface. Data acquisition will continue until fall 2006 when the mission officially ends.

1.2 Motivation for Simulations

Nowadays Physics have become very detailed and many of the problems arising are not analytically solvable. The computer provides a powerful tool to calculate complex phenomena in nearly arbitrary detail that, if possible at all, would have taken years of experimental assessment to measure. This is where computers are to be seen: In between of theory and experiment. On the one hand theoretical inputs are required to model the physical process. The governing laws have to be transformed from equations to algorithms. On the other hand the experiment is still needed in order to verify the simulation. One has
to be very cautious not to declare simulation outcomes to be the only truth without con-
siously rethinking and crosschecking the results. A computer will always remain a black
box where some things are thrown in and others are thrown out. In fact interpretation
of simulation data is often much more sophisticated than experimental data. The crucial
thing is that a simulation is a human-built thing. Humans do make mistakes; especially if
the degree of complexity is as high as in a computer simulation. Hence one should always
bear in mind that it is more than likely that a simulation contains errors.
However it is an undoubtable fact that computer simulations have become an essential
part in engineering and scientific investigations. Due to the enormous advancements in
information technology whole spacecraft, fusion reactors or airplane structures can be cal-
culated in “tabletop” simulations on available workstations. This speeds up investigation
and helps to understand interactions that have not been traceable before.
For the SMART–1 mission one of the most important things to learn are the interactions
and influences the exhausted plasma has on the spacecraft. These interactions require
high level plasma physics and do not permit satisfactory analytical treatment. In order
to investigate the physics of the Hall thruster plasma interactions SmartPIC has been
developed. This is the topic this work deals with.

1.3 Problem Definition

The main objective of SmartPIC is to predict the spacecraft floating potential $\Phi_{\text{SC}}$. Be-

\begin{table}[h]
\centering
\begin{tabular}{lll}
\hline
Parameter & Sign & Unit \\
\hline
Electron density & $n_e$ & m$^{-3}$ \\
Beam ion density & $n_i$ & m$^{-3}$ \\
Charge exchange ion density & $n_{\text{CEX}}$ & m$^{-3}$ \\
Neutral density & $n_n$ & m$^{-3}$ \\
Electron temperature & $T_e$ & eV \\
Ion energy (beam and CEX) & $E_i$ & eV \\
Plasma potentials & $\Phi_P$ & V \\
Spacecraft floating potential & $\Phi_{\text{SC}}$ & V \\
Backflow electron current density & $j_e$ & Am$^{-2}$ \\
Backflow ion current density & $j_i$ & Am$^{-2}$ \\
Thrust & $F$ & N \\
\hline
\end{tabular}
\caption{SmartPIC output parameters}
\end{table}

Previous versions have already been capable of predicting most of the parameters to
a far extent. However prediction of the spacecraft floating potential was difficult due to
some limitations arising from the computational design of the simulation. The solution for
static potentials caused by the solar array potential distribution and floating potential was
acquired only initially and adapted by the plasma potential depending on the ion density
(see Section 4.5.1). This is insufficient if changing floating potentials are considered.
Furthermore Debye shielding (Section 3.2.4) and breaking down of the quasineutrality
assumption in underdense regions above the solar array were not included. Finally the
formally utilized spatial resolution of 2.5 cm was insufficient for resolving interconnector
structures and potential distributions in the near field of the solar panels.
The three resulting objectives and requirements for enhancements being subject of this work are

- Implementation of a semi-adaptive multigrid with partially high spatial resolution.
  - The grid shall be of rectangular type.
  - The grid shall adapt to the solar array rotation as far as possible
  - Memory consumption shall be as low as possible and the simulation shall be able to run on a standard workstation PC.
  - The computational domain shall include at least half of the spacecraft main body and one solar array wing.

- Implementation of a fast multigrid solver for the Poisson equation
  - Speed of the solver shall allow instant solution for every ion time step
  - The potential shall be solved throughout the whole computational domain

- Development and implementation of an advanced electron fluid model allowing for a complete self-consistent electron density solution
  - The electron density shall be obtained without a-priori assuming quasineutrality throughout the domain
  - The plasma potential shall be calculated by the multigrid solver in accordance to ion and electron densities.
  - Calculation of the electron fluid shall still be possible on a standard workstation PC

The first two main requirements have been fulfilled completely. An advanced electron fluid model has been developed theoretically. Implementation has shown some stability and runtime issues not being resolved completely. This point is subject of future investigations.
Chapter 2

Technological Background

2.1 Plasma Diagnostic

Measurement of plasma parameters is a highly sophisticated field. Apparatus and methods have to be adapted to the experimental situation and the nature of the investigated plasma. Intrusive techniques raise the problem of disturbance to and interaction with the system. Recent advancements in optical methods for acquirement of density and temperature provide alternatives. Information on current measurement technology developments can be found exemplary in in [1] or [2].

In the current investigation only two classical plasma sensors have been utilized. These will be discussed subsequently.

2.1.1 Langmuir Probes

Langmuir probes (LP) (named after Irving Langmuir 1881-1957) can be utilized to obtain electron density $n_e$ and temperature $T_e$ data. Principally LP are intrusive sensors with the need to be positioned exactly at the place of interest. The measurement principle relies on the theory of floating potentials. The probe tip which is placed in the plasma consists of electrically conducting material (mostly Tungsten) which receives currents $I_e$ and $I_i$ for electrons and ions respectively. The tip represents the cathode of the measurement system. It is applied an external voltage $V_L$ relative to ground or, in space applications, to the spacecraft body. Depending on $V_L$ the net current to the probe will vary. Based on the theory given in Section 3.3.2 of this work the following relation can be derived for a single LP

$$I_L = \frac{A_L e}{4} \left[ n_i v_{Th,i} - n_e v_{Th,e} e^{\frac{e(V_P-V_L)}{k_B T_e}} \right]$$  \quad \text{for} \quad V_L < V_P

$$I_L = \frac{A_L e}{4} \left[ n_i v_{Th,i} e^{\frac{e(V_P-V_L)}{k_B T_i}} - n_e v_{Th,e} \right]$$  \quad \text{for} \quad V_L > V_P

Where $V_P$ depicts the plasma potential relative to ground, $A_L$ is the geometrical surface of the probe, and $v_{Th,ei}$ the mean value of thermic particle movement of electrons and ions respectively. Since for $V_L > V_P$ the ion current rapidly vanishes (sharp lower knee in Figure 2.1) and the electron current reaches its saturation value one can easily determine $I_i$ and the plasma potential $V_P$ from the tangents in the measured curve. One is left with four unknown variables here: $T_e$, $T_i$, $n_e$, and $n_i$. The assumption of quasineutrality
\( n_i = n_e \) in the plasma rules out \( n_i \). Furthermore thermal equilibrium requires \( T_e = T_i \). Finally the steepness of the LP curve gives the electron temperature

\[
T_e = e I_i \left. \frac{dV}{dT} \right|_{V_L=0}
\]  

(2.1)

Starting at the expression for the ion current \( I_i = e A_L n_e v_{Th,i} / 4 \) and \( v_{Th,i} = \sqrt{\frac{k_B T_e}{8 \pi m_i}} \) one can resolve for the electron density

\[
n_e = \frac{4 I_i}{e A_L} \left( \frac{k_B T_e}{8 \pi m_i} \right)^{-\frac{1}{2}}
\]  

(2.2)

These are the basics for measurements with single LP. In order to obtain the characteristic several measurements over a specific range of \( V_L \) are necessary. In addition all results depend on the plasma potential and grounding of the measurement circuit which cannot be measured directly. In practice multiple LP forming one differential probe are applied. Thus in the calculations \( V_P - V_L \) is replaced by the differential voltage \( V_{LD} \) between the probes. This eliminates the unknown reference ground potential. In principle the results and methods are the same mentioned above. Details and derivation can be found in [3].

### 2.1.2 Retarding Potential Analyzer

A retarding potential analyzer (RPA) is utilized to measure the ion energy in a plasma. RPA sensors consist of a ceramic pot with a metallic bottom plate which collects ions. Above this plate up to four metallic grids biased to different potentials select the ion energy and repel secondary electrons. In Figure 2.2 grid 1 is biased to spacecraft ground blocking field gradients propagating into the sensor. Grids 2 and 4 are tied to low negative potentials around \(-10 \text{ V}\) in order to repel primary and secondary electrons. Grid 3 selects the ion energy being applied a voltage of \( U_{RPA} = [0..U_{max}] \text{ V} \) where \( U_{max} \) usually takes values
of 400 − 600 V. $U_{RPA}$ decelerates the ions and, thus defines the measurement setpoint. Only particles with kinetic energies $m_i v_i^2 / 2 \geq e U_{RPA}$ are able to reach the collector.

The resulting ion current can easily be measured. A whole data set is generated by sweeping the setpoint $U_{RPA}$ from 0 V to $U_{\text{max}}$. Typical RPA current data takes an approximate $\tanh(E_i - E_{\text{max}})$ form (see Figure 2.3). Differentiation $dI/dE$ gives the relative intensity over the energy spectrum.

**Figure 2.2:** Schematic construction of a RPA sensor.

**Figure 2.3:** Typical current characteristic of a RPA probing a Maxwellian ion beam. Differentiation gives the relative intensity. The values for $U_{RPA}$ are chosen arbitrarily.
2.2 SMART–1 Geometry

2.2.1 Structure

The structure of SMART–1 is quite simple. It basically consists of a cubic main body \((l \times w \times h = 1110 \text{ mm} \times 1110 \text{ mm} \times 905 \text{ mm})\) with the thruster on top, and two solar array wings attached in \(\pm y\)-direction. The arrays consist of three panels, each 1740 mm in length and 960 mm wide. These are separated 90 mm by supporting structure elements. The wings are connected to the main body by extension arms (80 × 40 mm in diameter) of 900 mm length. Both extension arms are mounted separately pivotable around the \(y\)-axis which enables the arrays to follow the sun and provide maximum power. Rotation is performed by a motor in discrete steps of \(5^\circ\). The rotation angle \(\alpha\) is measured by the surface normal vector of the solar array relative to the plume vector which is parallel to the \(z\)-axis (see Figure 2.4).

The exact dimensions of SMART–1 can be seen in the Appendix. Due to the symmetry in \(y\)-direction the simulation includes only one half of the satellite (defined by \(y^+\)). Appropriate boundary conditions guarantee physical correctness (see Section 4.3.1).

2.2.2 Solar Array

The real structure of the solar arrays is rather complex. For use in the simulation some simplifications have been implemented which do not change basic details but “straighten” the geometry. An exact plan of the panel can be found in Appendix A.

The simplified structure is built up as follows. The two solar array wings are each divided into three panels of equal size. Each panel has 6 sections (in \(y\)-direction) which consist of three strings (in \(x\)-direction). The strings again are placed such that the voltage increases meander-shaped from 0 V to a maximum of 50 V along along 5 substrings. These are connected at their ends via interconnectors of 8 mm width. Supporting structures have metallic surfaces and are biased to spacecraft ground. Interconnectors are bare metallic (mostly Copper) and on the potential of adjacent solar cells. A view of the potential distribution can be seen in Figure 4.4. Solar cells are covered by non-conductive silicate coverglass of 150\(\mu\)m thickness. Potentials of the cells underneath the glass are propagated onto the surface nearly unhindered.

2.2.3 Geometrical input parameters

In addition to the physical input parameters given in Section 4 Table 4.1 the following geometrical parameters enter the simulation

![Figure 2.4: The rotation angle \(\alpha\) of the solar array is measured between the solar array normal vector \(n_{sa}, n'_{sa}\) and the positive \(z\)-axis.](image-url)
Figure 2.5: Simplified structure of the solar array as it was implemented in SmartPIC. All dimensions in [mm].

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Sign</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Domain size</td>
<td>$(DDS_x, DDS_y, DDS_z)$</td>
<td>(m,m,m)</td>
</tr>
<tr>
<td>Spacecraft dimension</td>
<td>$(DS_x, DS_y, DS_z)$</td>
<td>(m,m,m)</td>
</tr>
<tr>
<td>Offset of spacecraft body center</td>
<td>$SDO_z$</td>
<td>m</td>
</tr>
<tr>
<td>Solar array length</td>
<td>$DSA_y$</td>
<td>m</td>
</tr>
<tr>
<td>Solar array width</td>
<td>$DSA_x$</td>
<td>m</td>
</tr>
<tr>
<td>Solar array thickness</td>
<td>$DSA_z$</td>
<td>m</td>
</tr>
<tr>
<td>Solar array rotation angle</td>
<td>$\alpha$</td>
<td>°</td>
</tr>
<tr>
<td>Extension arm length</td>
<td>$DEX_y$</td>
<td>m</td>
</tr>
<tr>
<td>Extension arm width</td>
<td>$DEX_x$</td>
<td>m</td>
</tr>
<tr>
<td>Extension arm height</td>
<td>$DEX_z$</td>
<td>m</td>
</tr>
<tr>
<td>Thruster dimension</td>
<td>$(DT_x, DT_y)$</td>
<td>(m,m)</td>
</tr>
<tr>
<td>Thruster height relative to spacecraft surface</td>
<td>$DT_z$</td>
<td>m</td>
</tr>
<tr>
<td>Thruster inner cavity diameter</td>
<td>$r_i$</td>
<td>m</td>
</tr>
<tr>
<td>Thruster outer cavity diameter</td>
<td>$r_o$</td>
<td>m</td>
</tr>
<tr>
<td>Cathode position relative to thruster exit center</td>
<td>$(DC_x, DC_y, DC_z)$</td>
<td>(m,m,m)</td>
</tr>
<tr>
<td>Cathode diameter</td>
<td>$r_{cath}$</td>
<td>m</td>
</tr>
</tbody>
</table>

Table 2.1: Geometrical input parameters of the simulation
2.3 SMART–1 Instruments

The design included 7 main experiments providing a multiplicity of sensors and sub-experiments. In a plasma physics point of view two of these are of interest.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Abbrev.</th>
<th>Task</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electric Propulsion Diagnostic Package</td>
<td>EPDP</td>
<td>Monitoring of plasma parameters (potential, ion energy, density, temperature), and solar array sputter degeneration measurement.</td>
</tr>
<tr>
<td>Spacecraft Potential Electron and Dust Exp.</td>
<td>SPEDE</td>
<td>Measurement of electron density variations, electric potentials and plasma currents</td>
</tr>
<tr>
<td>Ka-Band TT&amp;C Experiment</td>
<td>KATE</td>
<td>X-band and Ka-band deep space telecommunication</td>
</tr>
<tr>
<td>Demo Compact Imaging X-ray Spectrometer</td>
<td>D–CIXS</td>
<td>X-ray spectrometry, Mapping of chemical components in lunar surface, 0.5 – 10 keV</td>
</tr>
<tr>
<td>SMART Infrared Spectrometer</td>
<td>SIR</td>
<td>Infrared spectrometry of the moon, geological science, 0.9 – 2.4 µm</td>
</tr>
<tr>
<td>X-ray Solar Monitoring</td>
<td>XSM</td>
<td>Long run X-ray spectrometry of sun and deep space sources</td>
</tr>
<tr>
<td>Advanced Moon micro-Imager Experiment</td>
<td>AMIE</td>
<td>High resolution multi-color and 3D imaging, Laser link to terrestrial base, data for autonomous navigation, 500 – 950 nm</td>
</tr>
</tbody>
</table>

Table 2.2: SMART–1 experiment packages

2.3.1 EPDP

The Electric Propulsion Diagnostic Package (EPDP) consists of one RPA, a LP, and a solar cell sample. The sensors are positioned at the edge of the top surface of SMART–1 facing the thruster while the solar cell sample is mounted on the -Z plane opposite to the thruster. Distance from the thruster axis is 550 mm in +Y direction and 150 mm from the thruster exit in -Z direction. Hence no direct measurement of beam ions is possible. The instruments capture plasma backflow data which is useful to estimate sputtering impact energies on surfaces.

The RPA acquires data about ion energy at its position which is well below 100 eV (in comparison to approximately 400 eV in the beam). Theory on this sensor is given in Section 2.1.2.

The single-ended Langmuir probe measures plasma parameters as potential, temperature, and electron density. Theoretical basis is given in Section 2.1.1. The purpose of the solar array sample is to monitor its performance over time in order to acquire representative degeneration profiles due to expected backflow contamination and lifetime limitations.

2.3.2 SPEDE

The Spacecraft Potential Electron and Dust Experiment (SPEDE) consists of two single-ended LP on the ±x planes. Each sensor is mounted on a 600 mm long boom.

SPEDEs objectives are electron (and ion density) measurements at either constant or
sweeping biasing voltage, investigation of plasma waves in a fast capture mode (10k samples per second) and data processing.

SPEDE not only measures plasma potential, density and temperature but enables also sensing of the spacecraft floating potential in conjunction with the EPDP device. This feature unfortunately has only been operational at the beginning of the mission and failed due to a damage in electronics.

The SPEDE LP sensor has been implemented as virtual probe in previous versions of the simulation but is not utilized in the current work.

2.4 In-flight Measurements

2.4.1 RPA Measurements

The position of the EPDP far out of the beam allows measurement of backflow ions. Data shows one major peak at 32-42 eV and one less pronounced peak around 55 eV. This indicates two species of CEX backflow ions: single, and double charged CEX particles. Measured intensities support this theory because the ratio of the two peaks (10–15%) correlates with the expected ratio of single to double charged ions of \(\approx 10\%\). 10–15% of the primary one.

Potential references on EPDP

The EPDP sensor is electrically floating with respect to the spacecraft. Hence RPA measurements are always offset by this differential voltage \(U_{f,EPDP}\). Measurements on SMART–1 have shown this voltage to vary from 11.5–18.5 V with the spacecraft floating potential. Figure 2.8(a) depicts these relative potentials for an example of \(U_{RPA,max} = 38\) V. Figure 2.8(b) gives an exemplary variation of the EPDP floating potential over a period of 5 days. Unfortunately data provided by ESA are very fragmentary and insufficient for determination of \(U_{f,EPDP}\) for the times where RPA measurement data is available. Hence in comparisons of simulation outputs with flight data upper and lower boundaries will be given.
2.4.2 Correlation of the Floating Potential with the Rotation of the Solar Array

In an early phase of the SMART–1 mission while the satellite still orbited Earth EPDP data analysis has shown a variation in the cathode reference potential $U_{crp}$. The effect was correlated with the discrete steps of the solar array rotation adapting to the suns position [5]. Due to a Fuzzy-Logic control algorithm the rotation is executed in discrete steps of $5^\circ$.

![Figure 2.7: EPDP RPA sample taken 2003-12-31 06:50:12. One main peak at 41 eV, diffuse backflow below 30 eV, long tail above the main peak and a little secondary peak at $\approx 55 – 60$ eV](image)

![Figure 2.8: Relative potentials on EPDP. a) depicts relations between different potential levels for an example of $U_{f,EPDP} = 18.5$ V. b) shows the measured variation of $U_{rp}$ and $U_{f,EPDP}$ for a differential voltage of 18.5 V.](image)
These steps have been the essential indicator to identify the correlation. If rotation had been performed continuously effects like enhanced secondary electron emission or variation in temperature depending on the position to the sun could not be excluded.

The cathode reference potential can be referenced to the spacecraft floating potential $\Phi_{sc}$ by

$$U_{sc} = -U_{crp} - 20.5 \text{ V}$$

(2.3)

This relation is proposed by the ESA plasma working group. It has been reported that a maximum change in $U_{crp}$ appears at rotation angles around $\alpha = 50^\circ$ [5]. Details can be seen in Figures 2.9 and 2.10. The most presumable explanation for the $50^\circ$ is that this position defines a maximum in attraction of electrons from the CEX domain above the solar array. The positive potential of the interconnectors shields the panels from high CEX densities. This widens the Debye length, and accordingly the effective electron collecting surfaces. In the $50^\circ$ position the solar array is on the one hand close to the plume, but on the other hand is at sufficient distance not to repel major parts of the CEX flow which acts as source of electrons. On higher angles up to $90^\circ$ slow ions are directed away from the array to a far extent. This theory is supported by the outcome of SmartPIC as will be discussed in Section 6.

Despite this obvious relation of the floating potential and the solar array rotation the measurements do not permit a general statement for the cause. Measurements exhibit phase offsets of nearly $\pm \pi/2$ when the potential variation is plotted over the rotation angle. To clarify the situation and explain the actual physical background of the of this effect a task for SmartPIC.
Figure 2.9: Correlation between the solar array rotation angle $\alpha$ and the cathode reference potential $U_{crp}$. The floating potential $V_f$ measured by EPDP is obviously depending on $\alpha$ too.
Figure 2.10: Correlation angle $\alpha$ and $U_{crp}$ on a more detailed scale. The discrete steps in $U_{crp}$ and the correlation to the $5^\circ$ steps of the array can be seen clearly.
2.5 Hall Thruster

Hall Thrusters have been developed in the 1950s–1970s in the USA, Japan, the former UdSSR, and Germany. Over 50 missions have been flown with this type of thrusters. Mainly they have been applied to control orbits of satellites for which they are referred to as Stationary Plasma Thrusters (SPT). In more recent missions as SMART–1 Hall thrusters have been utilized as main engines.

2.5.1 Function Principle

Hall thrusters are steady flow electromagnetic plasma thrusters. In contrast to pulsed engines this class works with static crossed E and B fields. Principally they are operated with quasineutral gas for which they are named plasma thrusters.

One could argue that ion acceleration is mainly due to an electrostatic field and, thus the type would be a standard ion thruster but several inherent properties are more likely to an electromagnetic accelerator. Hence it is a question of the point of view how to classify this type of thruster.

Hall thrusters are characterized by the coaxial cavity, surrounded by ceramic walls. On the bottom of the cavity neutral propellant, mostly heavy gasses with low ionization energy like Xe (12.13 eV) or Hg (10.44 eV), is inserted in axial direction through slits which are surrounded by the anode. The neutralizer is situated outside the thruster and represents the cathode. Electrons are emitted by the neutralizer, being accelerated by the electrical field into the cavity, creating an electron current $j_e$. A strong radial magnetic field turns the axial electron velocity into a tangential one by the $j_e \times B$ Lorentz force, forming a strong tangential ring current. Propellant is ionized by collisions with the hot electrons and accelerated by the electrical field gaining high exit velocities. The electron ring current

![Figure 2.11: Schematic construction and field configuration of a Hall thruster](image)
again interacts with the magnetic field forcing exhaust of electrons. Plasma expelled is almost completely neutral.

When reviewing this function principle in detail some conditions for efficiency and limits for thrust and power values appear. When entering the zone of high magnetic field the electrons start to gyrate perpendicular to the $\mathbf{B}$ field lines according to Equation (3.2.1). This produces a drift velocity $v_D = \frac{E \times \mathbf{B}}{B^2}$ in tangential direction. The resulting ring current is essential for ionization. If the Hall parameter is too low ($\beta_H \ll 1$) the gyration movement cannot form and ionization efficiency will drop. Ions observe gyration too. Due to their much higher mass their Lamor radius (3.20), and hence the time for one gyration cycle, is much bigger than that of the electrons. According to that they cover only a small fraction of a full gyration circle within the thruster while being expelled. Nonetheless the drift movement generated by ion gyration accounts for an ion ring current which accounts for an additional thrust component.

Detailed assessment of the theoretic background of steady magnetic and ion type thrusters is given by [6]. More compact descriptions are found in [7], and [4]. Several numerical models have been developed for simulation of internal processes ([8], [9]) as well as the plume ([10], [11], [12], et al).

### 2.5.2 Characterization

This type of thruster, despite being complex in design and detailed theory, comes up with some really outstanding advantages in performance. As for all electromagnetic engines the space charge limitation familiar with pure electric thrusters which limits the energy being transmitted to the plasma by the field, is not existent due to charge neutrality of the propellant in the cavity. Second high specific impulses of typically 1,500s are combined with short length design and moderate power consumption (some 100 W for station keeping, up to 2 kW for application as main engine). Total effectivity reaches 30 – 50% depending on the power level.

Main lifetime constrictions are erosion of ceramic material at the thruster exit due to fast ions and wearing down of the cathode. Typical lifetimes are 500 – 10,000 h.

The beam of a Hall thruster has a divergence of around 45° with a strong density gradient from the center to outer regions. Axial exit velocities are around 10 km s$^{-1}$. Radial velocities are smaller by a factor in the range [1..2].

### 2.5.3 PPS-1350 Hall Thruster

This thruster is a French development by SNECMA. The design is based on the well approved Russian SPT-100, adapted for higher powers and thrust levels. The PPS-1350 has been designed for application as main engine for the European moon mission SMART–1. Characteristic data is summarized in the following table ([10], [13]).
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Propellant</td>
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<td>Xe</td>
</tr>
<tr>
<td>Thrust</td>
<td>mN</td>
<td>70</td>
</tr>
<tr>
<td>Mass flow</td>
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<tr>
<td>Specific impulse</td>
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<td>Total efficiency</td>
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<td>51</td>
</tr>
<tr>
<td>Maximum power</td>
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<td>1500</td>
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<td>Nominal power</td>
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<td>Lifetime</td>
<td>h</td>
<td>7000</td>
</tr>
<tr>
<td>Acceleration voltage</td>
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</tr>
<tr>
<td>Plasma current</td>
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<tr>
<td>Ionization efficiency</td>
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<td>95</td>
</tr>
<tr>
<td>Divergence angle</td>
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</tr>
<tr>
<td>Inner cavity diameter</td>
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<td>56</td>
</tr>
<tr>
<td>Outer cavity diameter</td>
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</tbody>
</table>

**Table 2.3:** Parameters of the PPS-1350 Hall thruster
Chapter 3

Physical Background

Electrical propulsion and plasma theory is based on a wide array of fields. Thermodynamics, electrodynamics, kinetics in classical and relativistic domains, material sciences, and chemistry all are necessary to describe the manifold effects and correlations. Hence a sweep over, at least the most important aspects, of all these fields is necessary to form the basis for analytic description and modeling of the occurring plasma effects.

3.1 Thermodynamic Theory

When starting to describe plasmas one has to start from the classic theory of gasses. Basic definitions and connections will be given in 3.1.1. Inclusion of time dependence leads to kinetic gas theory and continuity equations of multiple order in 3.1.2. These form the basis for modeling of plasma fluids.

3.1.1 Classical Gas Theory

Classical gas theory deals with the statistical description of the macroscopic behavior of a great number $N$ of particles called a system based on classical mechanics. Due to some basic assumptions the validity of the theory is bound to the following requirements.

1. The number $N$ of particles in the system has to be huge.
   \[ N \gg 1 \]

2. The De-Broglie wavelength $\lambda_{DB}$ has to be small compared to the mean distance of two particles.
   \[ \frac{\hbar}{2\pi mv} \ll d = \left( \frac{N}{V} \right)^{\frac{1}{3}} \]

3. The occurring thermal particle velocities have to be small compared to the speed of light.
   \[ v \ll c \]

The first condition arises from the validity and representativeness of statistical mean values that are in general defined as $\langle a \rangle = \frac{1}{N} \sum_{i=1}^{N} a_i$ for an arbitrary variable $a(i)$. The second limit is argued by the influence of quantum mechanical effects as the tunnel effect which in a classical point of view disturb the system by altering probabilities for a change of state. These effects arise only for characteristic distances smaller than the De-Broglie wavelength. At least the requirement for a maximum velocity comes from the special
theory of relativity that converges to classical mechanics for speeds at least two orders below the vacuum speed of light.

Thermodynamic as it is understood nowadays represents the statistical limit theory of quantum mechanics. Microscopic quantum effects are governing the macroscopic behavior of a system which can be described statically in parameters as pressure, temperature, volume, specific heats, ... and dynamically in terms of kinetic flow vector fields that again are influenced by macroscopic parameters as the Reynolds number, viscosity, diffusion coefficients and many others.

**Thermodynamical Definitions**

This section is intended to give short but clear definitions of the terminology that are used throughout this work.

**Ideal Gas** The ideal gas is a system of $N$ particles of equal type that are enclosed in a finite volume $V$ and for which the following holds

- Interactions are rare, so every particle moves in good approximation undisturbed through space and no interaction energy must be taken into account.
- The level of interactions is high enough to allow energetic equilibrium throughout the system.
- Particles feature only translational degrees of freedom.

In nature gasses behave like ideal gasses for the limit of low density.

**Thermal Equilibrium** This expression refers to a system state that is classified by its time independence. The thermal equilibrium is the state of a system left undisturbed for the limit of $t \to \infty$. Thus it is the state with the highest probability to be reached.

**Distribution function and phase space** Thermodynamical calculations are done in the $6+1$ dimensional phase space $\mu(x_i, v_j, t)$ where $i, j \in \{1, 2, 3\}$. In other words the phase space is built up by three spatial coordinates $x_i$, three velocity coordinates $v_j$ and the time $t$. Note that the spatial variables are independent of the velocity coordinates and vice versa. According to that definition one can deal with probabilities $P(x, v)$ for a particle to be in a specific volume element $\Delta \Omega([x + \Delta x], [v + \Delta v], t)$. By demanding

$$P(x, v \epsilon \Delta \Omega(x, v, t)) = \int_{\Delta \Omega} d\Omega p(x, v, t) \quad (3.1)$$

one defines a probability density $p(x, v, t)$ which subsequently gives the distribution function

$$f(x, v, t) = Np(x, v, t) \quad (3.2)$$

which is an expression for the particle density in phase space. So the distribution function $f(x, v, t)$ gives the mean number of particles expected to be found in a phase space element $\Delta \Omega = f ([x, x + \Delta x], [v, v + \Delta v], t)$. Furthermore $f$ fulfills

$$n(x, t) = \int_{-\infty}^{+\infty} d^3v \, f(x, v, t) \quad (3.3)$$

the number density distribution in spatial space. For an ideal gas assuming spatial homogeneity (or thermal equilibrium), isotropy, and independence among the velocity
components, one can derive \[14\] the well known *Maxwell velocity distribution*

\[
f_M(v) = n \left(\frac{\beta}{\pi}\right)^{-\frac{3}{2}} e^{-(v^2 \beta)}
\]  

(3.4)

The parameter \(\beta \in \mathbb{R}\) is left undefined for the first. Later on it will be replaced by \(\beta = \frac{m}{2k_B T}\).

---

**Figure 3.1:** Maxwellian velocity distribution. The function is symmetrically in \(v\)

---

**Inherent energy and temperature** Since the mean particle velocity must yield

\[
\langle v \rangle = \frac{1}{n} \int_{-\infty}^{+\infty} dv v f(v)
\]  

(3.5)

it does not depend on the spatial direction. Hence the total kinetic energy of the system is not directed. This is referred to as the *inherent energy* or *thermal energy* of the system.

Its expected value for a particle \(p\) is expressed by

\[
E_{p,\text{Th}} = \frac{m_p}{2} \langle (v - \langle v \rangle)^2 \rangle
\]

Inserting (3.5) and the Maxwellian distribution for an ideal gas little calculation \[14\] gives

\[
E_{p,\text{Th}} = \frac{3}{2} \frac{m_p}{2} \beta
\]

In order to resolve the undefined parameter \(\beta\) one simply defines \(\beta = \frac{m_p}{2k_B T}\) with the new parameter \(T\) which is proportional to the thermic energy and a constant \(k_B\). The value for \(k_B\) is justified to fit \(T\) by the historical K-scale. \(T\) is called *temperature* and the thermal energy takes the form

\[
E_{p,\text{Th}} = \frac{3}{2} k_B T = \frac{3}{2} m_p \langle v^2 \rangle
\]  

(3.6)

---

20
Mean Velocities  As can be seen from Figure 3.1 \( \langle v \rangle = 0 \). But the expectation value \( \langle v^2 \rangle = \langle (v - \langle v \rangle)^2 \rangle \) does not vanish. One defines the thermal velocity

\[
v_{\text{Th}0} = \sqrt{\langle v^2 \rangle} = \left( \frac{m}{2\pi k_B T} \right)^{\frac{1}{2}} \int_{-\infty}^{+\infty} dv \, v^2 \, e^{-\frac{mv^2}{2k_BT}} = \sqrt{\frac{3k_B T}{m}}
\]

which would be characteristic if all particles had exactly the kinetic energy that equals the mean inherent energy of the gas. This would require \( f(v^2) = \delta(v^2_{\text{Th}0}) \). Hence the mean velocity including the Maxwell distribution is much more representative.

\[
v_{\text{Th}} = \langle v \rangle = \frac{2}{n} \int_0^{\infty} d^3v \, |v| \, f_M(|v|) = \sqrt{\frac{8k_B T}{\pi m}} \quad (3.7)
\]

Pressure and the Equation of State  Pressure is the cumulative force a system exerts on a normalized area element of its constricting boundary. This force is, according to (3.5) and (3.4) proportional to the temperature. The pressure \( p \) can be expressed as

\[
p = \frac{1}{A} \int_A dP \frac{dt}{dt} \quad \text{with} \quad dP = 2m\langle v^2 \rangle f(v) \frac{(A \cdot v)}{|v|} dv dt \quad (3.8)
\]

for a total boundary area \( A \) with appropriate normal vector \( A \). \( P \) is the directed change in momentum for a particle with velocity \( v \) being reflected by \( A \). Evaluation and insertion of the mean velocity depending on the temperature (3.5) yields

\[
p = \frac{mn\langle v^2 \rangle}{3} \quad (3.9)
\]

and with Equation (3.6) finally

\[
p = \frac{Nk_B T}{V} = nk_B T \quad (3.10)
\]

the equation of state for an ideal gas.

3.1.2 Boltzmann Equation

Boltzmann’s equation forms the basis for the kinetic calculation of gases and fluids. It describes the time evolution of a velocity distribution function \( f(x, v, t) \) in the 6 + 1-dimensional phase space \( \mu(x_i, v_j, t) \). \( f \) by definition fulfills the equality

\[
\int_0^{\infty} d^3v f(x, v, t) = n(x, t)
\]

As shown in Section 3.1.1 the distribution function in practice for thermal equilibrium is assumed to be Maxwellian. If the temperature is neglected stating \( T = 0 \), \( f(v) \) reduces to a delta distribution around a speed \( v_0 \) that is chosen to satisfy the current problems conditions. The following famous equation published by Ludwig Boltzmann 1872 completely describes the thermodynamical evolution of a gas penetrated by external forces \( F \) of arbitrary type. Its derivation and discussion can be found in most undergraduate and graduate textbooks ([14], [15]).

\[
\frac{\partial f}{\partial t} + v \nabla_x f + \frac{F}{m} \nabla_v f = \left( \frac{\delta f}{\delta t} \right)_c \quad (3.11)
\]

This is the Boltzmann equation which represents a continuity equation in \( \mu \). The first term describes the temporal change in the distribution, while the second and third term
represent fluxes. The term on the right side is called *collisional term* and represents a source. The latter is causing serious problems in solving Equation (3.11). Numerical solution of the full Boltzmann equation requires a huge computational effort and is not feasible in reasonable times. Thus one has to make assumptions in order to simplify the problem and gain a new relation that is, at least numerically, practically solvable. When seeking a simplified set of equations in general there is an approach known as the *momentum method*. One multiplies (3.11) by a specific factor $g$ and integrates over the velocity space. $g$ represents a momentum expression of orders 1, 2, 3, \ldots. Accordingly one gains an equation for conservation of a momentum of appropriate order to $g$. The following discussion is written in a plasma point of view. Hence most expressions for source and other terms are specialized. Missing definitions originating from plasma physics can be read in Section 3.2.

Let $g = 1$ then follows

$$\frac{\partial n_\alpha}{\partial t} + \nabla_x (n_\alpha v_\alpha) = 0 \quad (3.12)$$

the *continuity equation* for each constituent $\alpha$ of the plasma. If the collisional term is not neglected it has to represent a source for charged particles. Such a term in general has the form $R = n_i n_e C_{ei}$ where $C_{ei}$ is a statistical ionization source factor provided by transport theory. Models for calculation of $C_{ei}$ can be found in [16].

Physically Equation (3.12) relates the density to the particle flux $\Gamma_\alpha = n_\alpha v$. The velocity $v$ is unknown and requires determination by a first order momentum equation which will follow next.

In the second case, $g = mv$ ,usually two simplifications are made to Equation (3.11) which will be described briefly. First the fluid velocity $v$ is split into a common part $u = \langle v \rangle$, where $\langle \cdot \rangle$ represents the statistical mean value, and a stochastic randomized part $v_r$ which equals the thermic movement. Thus

$$v = u + v_r \quad \text{and} \quad \langle v_i v_j \rangle = u_i u_j + \langle v_r,i v_r,j \rangle$$

Second the stress tensor $P$ is split into its symmetric trace part $1p$ which holds the pressure coefficients $p_{ii}$ and the rest $\pi$ which represents the non-isotropic coefficients. The latter one is often referred to as the *viscosity tensor*. Hence one can state

$$P = 1p + \pi$$

If isotropic behavior is assumed the pressure tensor can be reduced to the scalar pressure $p$ which in advance can be derived from an equation of state $p = p(n, T)$. The viscosity tensor can be omitted in most cases. Including these considerations the momentum method for the first order gives

$$m_\alpha n_\alpha \frac{du}{dt} + \nabla_x p_\alpha + \nabla_x \pi - e_\alpha n_\alpha (E + u \times B) = R \quad (3.13)$$

the *equation of motion*. $e_\alpha$ depicts the charge of constituent $\alpha$. On the right side $R$ defines the momentum transfer in the fluid. It is defined as

$$R = \int d^3 v \ m v \left( \frac{\delta f}{\delta t} \right)_e$$

Again, explicit calculation of $R$ can only be performed with the help of transport theory. One simple approximation to this term can be given by the *Krook friction term* defined by

$$R_{\text{Krook}} = n_e m_e \nu_{ei} |v_i - v_e| \quad (3.14)$$
with the electron–ion collision frequency \( \nu_{ei} = n_i \sigma_{ei} |\mathbf{v}_i - \mathbf{v}_e| \) and \( \sigma_{ei} \) being the total electron–ion collision cross section which has either to be determined by experiment or be given by the theory of coulomb scattering. This model despite of its simplicity is very accurate for low temperatures \( k_B T_e < 1 \text{ keV} \) which is generally the case for the far field of Hall thruster plumes. The most challenging task is to find the right values for \( \sigma_{ei} \) which is highly nonlinear in \( T_e \).

![Figure 3.2: Total \( e^- \) cross section in Xe taken from [17]](image)

For completeness one more thing has to be mentioned. The total derivation \( d/dt \) has to be taken in the phase space \( \mu \) where the velocity and acceleration terms have to be taken into account. One defines the \textit{substantial derivation}

\[
\frac{d}{dt} = \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u}
\]  

(3.15)

which accounts for contributions of flow effects of \( v_i \) in \( \mu \).

Physically (3.13) relates the fluid velocity to forces caused by stress and electromagnetic fields. In classical fluid theory the equation of motion takes a slightly different form and is referred to as the \textit{Navier Stokes equation}.

Again in equation (3.13) there is an unknown variable: The stress tensor \( \mathbf{P} \) or, in the simplified case, the scalar pressure \( p \). These have to be determined by a second-order momentum equation.

Multiplying Boltzmanns equation (3.11) by \( mu^2/2 \) and integrating over the velocity space results in the \textit{energy equation}

\[
\frac{3}{2} n_a k_B \frac{dT}{dt} - \mathbf{P} (\nabla \cdot \mathbf{v}) - \nabla \cdot \mathbf{q} = Q
\]  

(3.16)

Where \( Q \) is the amount of heat induced by collisions in the gas. It is again defined by an
integration of the momentum and the collisional term

\[ Q = \int d^3v \frac{m v^2}{2} \left( \frac{\delta f}{\delta t} \right)_c \]

As in the other momentum equations (3.12) and (3.13) a new unknown variable appears: the heat flux \( q \) which can be defined as

\[ q_\alpha = \int d^3v \frac{m v^2}{2} v_r f \]

Theoretically this would require a higher order equation which again yielded another unknown and so on. Usually the process is cut off at this stage because the heat flux can be neglected in most cases. Equations (3.12), (3.13), and (3.16) together with the four Maxwell equations provide a basis for calculation of a plasma in a fluid point of view.

### 3.2 Plasma Physics

Plasma – the 4th state of matter has not been paid much attention until the early twentieth century when glow discharges became important in technical applications for radio transmissions. Due to the absence of plasmas within the Earth’s lower atmosphere (with the exception of arcs in thunderstorms) there was only little motivation to investigate this kind of state. In fact most of the matter in the universe is present in the form of a plasma. As soon as we reach for the higher layers of our atmosphere and take a look into space we are confronted with plasmas of various kinds. Dense plasmas in the ionosphere, the sun’s flares, stellar and interstellar gas clouds and flows, nebulae, galaxies.

However, man started to show massive interest in plasmas in the 1940s when the idea of controlled nuclear fusion became popular. Since then extensive theoretical and practical investigations have revealed many of the interesting and unique properties of plasmas not being shown by any other state or material.

This section is intended to give a brief overview of the definitions and physics needed for description of the model presented in Section 4. First some basic plasma variables will be introduced. These in advance will be utilized to state classification criteria. Finally a short overview of the standard plasma models is given.

#### 3.2.1 Plasma Parameters

**Debye length**

The Debye length of a Plasma defines the range an electrostatic perturbation can influence the properties of a plasma. Its derivation reveals important aspects of the underlying physics which will be discussed in detail in Section 3.2.4. For completeness the definition of this parameter is given.

\[ \lambda_D = \sqrt{\frac{\varepsilon_0 k_B T_e}{n_e e^2}} \]

**Plasma parameter**

This parameter simply quantifies the number of particles in a sphere with the radius of one Debye length. \( N_D = \frac{3}{4} \lambda_D^3 \pi n \)

**Plasma frequency**

If a disturbance of electrostatic nature perturbs a plasma electrons are accelerated
much more than ions due to their little mass. So the electrons try to counterbalance the disturbance. When the equilibrium position is reached the electrons move a little further due to inertia. This overshooting causes a continuous oscillation of electrons around their equilibrium positions. These oscillations have the plasma frequency $\omega_{pe}$

$$\omega_{pe} = \sqrt{\frac{n_e e^2}{m_e \epsilon_0}} \quad (3.18)$$

One might define a frequency $\omega_{pi}$ for the ions in the same way. This frequency is of importance when plasma waves are subject of investigation but it will not be used further in this work.

**Cyclotron frequency**

When external magnetic fields are applied to a plasma the charged particles start to gyrate. This circular movement is the basis for some plasma phenomena not appearing in uncharged gases. The so called *drift movements* which are directed orthogonal to the $E$ - and $B$ fields cause diffusion and, more general, transport of particles. Every inhomogeneity in the external fields, pressure or density causes additional drifts. Together these movements lead to non-classical transport phenomena. One prominent example for these drifts is the particle movement in the *Van Allen belts* in the upper atmosphere. Charged particles from the sun are caught by the Earths magnetic field. Depending on their charge these particles move north or south along the field lines. In doing so they gyrate and, hence observe a drift parallel to the equator. In that case the drift is not caused by an $E \times B$ force but by the cross product of the magnetic and gravitational field. However, particles are reflected when reaching polar regions where the more dense field acts like a magnetic mirror. Particles of higher kinetic energy are not mirrored and follow the polar field lines down into the atmosphere causing the famous auroral lights.

The gyrofrequency or cyclofrequency is defined as

$$\omega_{ce} = -\frac{eB}{m_e} \quad (3.19)$$

From this definition the *Lamor radius* for gyration movement can be extracted to

$$r_c = \frac{v_\perp}{\omega_{ce}} \quad (3.20)$$

where $v_\perp$ is the velocity component lying in the plane of the gyration cycle ($v_\perp = |v - v \cdot \omega_{ce}|$).

**Collision frequency**

Collisions in gases are statistical processes. Thus only mean values of the microscopic parameters can be given. Such is the collision frequency. Its derivation from thermodynamic theory and the form it takes depends on the assumptions being made. Generally the collision frequency can be expressed as

$$\nu_{ci} = \sum_j n_j \Delta v_{Th,ij} \sigma_{ij} \quad (3.21)$$

which gives the total collision frequency for a particle type $i$, $\Delta v_{Th,ij}$ depicts the mean relative velocity to particle species $j$, and $\sigma_{ij}$ is the collision cross section. The latter one brings difficulty to this expression. It strongly depends on the type of particles, temperature, and the degree of ionization. For fully ionized plasmas so called Coulomb collisions govern the cross sections. In that case not geometrical cross section areas are of
importance but the effective area of influence between two charged particles. The radius \( r_{\sigma C} \) of a circular cross section can be obtained by equalling kinetic energy of the particles with potential energy in the electric field of the collision opponent. The effective area, and further the Coulomb collision cross section can be expressed by

\[
\sigma_C \approx r_{\sigma C}^2 \pi = \frac{Z^2 e^4}{16\pi \varepsilon_0^2 m_e^2 v_{Th,e}^4}
\]

Inserting this expression into (3.21) gives the electron-ion collision frequency \( \nu_{ei} \).

The approximation to equalize Coulomb potential and kinetic energy introduces an error which is corrected by introducing the Coulomb logarithm \( \ln \Lambda = \ln \left( \frac{b_{\text{max}}}{b_{\text{min}}} \right) \) with the minimum collision parameter \( b_{\text{min}} \) determined by the kinetic energy of the colliding particles and \( b_{\text{max}} \) the maximum collision parameter set to the Debye length \( \lambda_D \). Exact derivation bases on the Focker-Planck Equation (3.39) and can be found in [14] and other standard textbooks on thermodynamics and plasmas.

\[
\langle \nu_{ei} \rangle = \sqrt{\frac{2}{\pi^3 m_e T_e^3}} \frac{n_i Z^2 e^4 \ln \Lambda}{12 \varepsilon_0^2} (3.22)
\]

This represents the mean electron ion collision frequency for a plasma with Maxwellian velocity distribution.

For partially ionized gasses collisions between charged particles and neutrals govern the behavior. Spitzer derived an expression for the electrical resistivity which is known as the Spitzer resistivity for plasma.

\[
\eta_S = \frac{1}{64\pi \varepsilon_0 \omega_{pe}} \frac{\ln \Lambda}{\Lambda} (3.23)
\]

With \( \eta = \frac{m_e v_c}{n_e e} \) the collision frequency can be calculated.

**Hall parameter**

Searching for a measure for the collisionality of a plasma and anticipating a classification requirement discussed in the next section (3.2.2) one can state the following: In order to allow plasma effects like waves or particle gyration to form out, the plasmas collision frequency \( \nu_c \) has to be much smaller than the characteristic frequency of the effects. Since electron gyration governs most or the characteristics of a plasma it is \( \omega_{ce} \) that is taken as a reference. The ratio

\[
\beta_H = \frac{\omega_{ce}}{\nu_c} (3.24)
\]

is called the Hall parameter. If \( \beta_H \gg 1 \) electrons gyrate nearly unhindered and drift movements \( E \times B \) form out. If on the other hand \( \beta_H << 1 \) the plasma is called collisional and particles mainly follow the \( E \) field lines. Since \( \omega_{ce} \propto B \) the hall parameter can only be defined if a magnetic field is present. Thus the definition of collisionality needs to be extended which will be done in the next section.

**3.2.2 Classification**

Principally a plasma is an electrically neutral gas that is at least partially ionized and capable of collective behavior.

This rough definition already includes the most important facts to characterize a plasma: neutrality, ionization, and collective behavior. These properties depend on each other and are the main reason for all the major plasma effects. The classification when a fluid or gas is a plasma or not can be done using three basic conditions
1. The number of particles in a Debye sphere has to be much greater than 1.
\[ N_D \gg 1 \]

2. The system dimension has to be much greater than the Debye length.
\[ L \gg \lambda_D \]

3. Collisions must not govern the behavior of the plasma.
\[ \nu_c \ll \omega_{pe} \]

These conditions can be understood as follows. The first one comes from the validity condition for statistical treatment of gases already discussed in Section 3.1.1. The second requirement is reasoned by the fact that waves (both, longitudinal density waves, and electromagnetic waves of transverse as well as longitudinal nature) can form in a plasma. If the system dimension \( L \) is too small compared to the characteristic length of effects in the plasma (represented by the Debye length) waves do not interact with the plasma at all or are just randomly scattered. Hence the formation of waves in general cannot take place in a plasma of \( L \ll \lambda_D \) and this contradicts the requirement of the existence of plasma waves.

The condition of a low collision frequency again attaches at this point. If collisions between electrons and neutrals or ions damp out waves no plasma oscillations are possible. In contrast to the definition of \( \beta_H \) in the former section not the electron gyrofrequency but the plasma frequency is taken as a reference which is independent of magnetic fields.

In addition the requirement for a globally neutral system implies again that the number of particles in the system must be large enough in order to provide \( n_e = n_i \), charge neutrality. This is called quasineutrality. Quasi because of local fluctuation caused by thermal movement and oscillations that cause the build-up of temporal local charge domains. Globally the plasma always tends to the most neutral state possible. Detailed discussion of this thematic can be found in Section 3.2.4.

### 3.2.3 Simplified Plasma Fluid Models - a short Review

In this section three well known models are presented in a brief and informative way. The first one is known as the cold plasma model. It neglects the stress tensor \( \mathbf{P} \) in (3.13) which corresponds to the assumption \( T = 0 \). The model applies in isotropic non-collisional plasmas of low density with magnetic fields as they appear in the magnetosphere or under special circumstances in fusion reactors.

Since thermal spreading of the distribution function cannot take place it is reduced to \( f_\alpha(v, x, t) = \delta(v - u_\alpha, x, t) \). The system is described completely by the continuity equation (3.12) and the equation of motion (3.13). For the latter one the friction or collisional term \( \mathbf{R} \) is often neglected too.

Another simple model is the so called warm plasma model which assumes isotropy (\( \pi = 0 \)), no collisions (\( \mathbf{R} = 0, \mathbf{Q} = 0 \)), and adiabatic behavior (\( \mathbf{q} = 0 \)). These assumptions lead to a simple set of equations describing the system completely. The continuity equation (3.12), the equation of motion which reduces to
\[
m_\alpha n_\alpha \frac{dv}{dt} + \nabla_x p_\alpha - e_\alpha n_\alpha (E + v_\alpha \times B) = 0
\]
and the adiabatic energy equation which takes the same form as in classical gas theory
\[
p_\alpha n_\alpha^{-\gamma} = \text{const} \quad \text{or} \quad \nabla p_\alpha = k_B T_\alpha \gamma \nabla n_\alpha \quad \text{with} \quad \gamma = \frac{C_p}{C_v}
\]
The ratio of the specific heats $C_p$ and $C_v$ takes values between $3/3$ and $5/3$. Finally one of the most prominent models for describing plasma fluids, the *magneto-hydrodynamic (MHD) model* should be introduced. This model takes advantage of some basic plasma properties and uses them to simplify without neglecting too much. Principally a collisional isotropic adiabatic behavior is assumed. In addition to that the plasma is treated as one single fluid and no further distinction between the different plasma constituents is made. This can be reasoned by the effect of ambipolar diffusion which permits different diffusion rates for each particle type due to the electrostatic coupling of ions and electrons. Executing this thought one has to define mean variables

$$
\rho_{mM} = n_e m_e + n_i m_i \\
u_M = \frac{u_e n_e m_e + u_i n_i m_i}{\rho_m} \\
\rho_M = n_e e + Z n_i e_i \\
j_M = e_e n_e \left( u_e - \frac{n_i}{n_e} u_i \right)
$$

The momentum equations (3.12), (3.13), and (3.16) take the form

$$
\frac{\partial \rho_{mM}}{\partial t} - \nabla_x (\rho_M u_M) = 0 \\
\rho_{mM} \frac{d u_M}{d t} + \nabla_x p_0 - \rho_M e - j_M \times B = 0 \\
\rho_M p^{-\gamma} = \text{const}
$$

This model is often applied in numerical calculations in fusion physics and space plasma simulations. The main restriction to the MHD model is the validity of the ambipolar assumption which is the basis for the one–fluid approach. When occurrence of high electrical field gradients is expected, quasineutrality can be broken and the ambipolar assumption is no longer valid. This thematic will be discussed in detail in Section 4.5.

One further relation has to be introduced which gained high popularity in plasma physics: the *Boltzmann relation* or *Boltzmann law* (not to be confused with the Boltzmann equation (3.11)). Basically this relation is a strongly simplified abundant of the equation of motion (3.13) that is resolved for the electron density or the electric potential. Starting from the stationary part of the Equation (3.13) neglecting magnetic fields, ionization and recombination effects, and collisions the isotropic pressure balances the electric forces

$$
e n_e E = \nabla p
$$

Eliminating further $p$ by the equation of state for an ideal gas (3.10), assuming thermal equilibrium and introducing the scalar electric potential $\Phi$ one obtains

$$
\varepsilon \nabla \Phi = \frac{T_e}{n_e} \nabla n_e
$$

which has the well known exponential solution

$$
n_e = n_{e,0} e^{-e (\Phi - \Phi_0) / k_B T_e} \quad \text{or} \quad \Phi = \frac{k_B T_e}{\varepsilon} \ln \left( \frac{n_e}{n_{e,0}} \right) + \Phi_0 ,
$$

the Boltzmann relation. Setting the equilibrium density $n_{e,0} = n_i$ and the free space potential $\Phi_0 = 0$ V or alternatively a reference point of known $n_{e,0}$ and $\Phi_0$ one is able to calculate the plasma potential $\Phi$ from the known ion density and the electron temperature.


3.2.4 Debye Shielding

The effect of Debye shielding is one of the most important features that distinct plasma from other states of matter. It directly shows the collective behavior of the whole system reacting on a local disturbance.

Principally a plasma can be modeled as a collection of charged particles of at least two types, ions and electrons, and neutrals. Since Coulomb forces grow dramatically for even little deviations from charge neutrality the plasma always tends to the most neutral state possible.

In order to derive a relation for the local potential distribution around a disturbance one considers a test charge \( Q \) at some point \( \mathbf{r}_0 \) in the plasma. Remembering the Boltzmann relation (3.25) one obtains for the total charge density \( \rho(\mathbf{r}) \) in the vicinity of the test charge

\[
\rho(\mathbf{r}) = e[n_i(\mathbf{r}) - n_e(\mathbf{r})] + Q\delta(\mathbf{r}_0)
\]

where the equilibrium plasma density \( n_0 = n_i = n_e \) for the case of neutrality has been introduced. Inserting this charge density into Poisson’s equation in spherical coordinates results in

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Phi(r)}{\partial r} \right) = -\frac{en_0}{\varepsilon_0} \left[ e^{\Phi(r)} e^{\Phi(r)} - e^{-\Phi(r)} e^{-\Phi(r)} \right] + Q\delta(r_0)
\]

with \( r \equiv |\mathbf{r}| \). This nonlinear differential equation cannot be solved easily and not at all in a purely analytic way. For \( e\Phi \ll k_BT \) the right side can be expanded into Taylor series around \( r_0 \).

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Phi(r)}{\partial r} \right) = -\frac{en_0}{\varepsilon_0} 2 \left[ \frac{\Phi(r)}{k_BT} + \ldots \right] + O\left( \frac{\Phi(r)}{k_BT} \right)^3 + Q\delta(r_0)
\]

When breaking after the linear term, rearranging and introducing the Debye length (3.17) one obtains

\[
\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Phi(r)}{\partial r} \right) + \frac{2}{\lambda_D^2} \Phi(r) = Q\delta(r_0)
\]

The ansatz \( \Phi(r) = F(r)/r \) reduces the problem to

\[
\frac{\partial^2 F(r)}{\partial r^2} + \frac{2}{\lambda_D^2} F(r) = Q\delta(r_0)
\]

This equation has the general solution

\[
F(r) = C_1 e^{\frac{\sqrt{2}}{\lambda_D}} + C_2 e^{-\frac{\sqrt{2}}{\lambda_D}}
\]

with the constants \( C_1, C_2 \) to be adapted to the problem. Since the potential is expected to tend to 0 for \( r \rightarrow \infty \) \( C_1 = 0 \). \( C_2 \) can be evaluated taking advantage of Gauss’ theorem.

Integrating over a ball \( B \) with the boundary sphere \( S \) of radius \( a \) the theorem states that

\[
\int_B dV \Delta \Phi(r) = \int_S df \frac{\partial \Phi}{\partial r} = \frac{Q}{\varepsilon_0}
\]

Inserting the solution for \( \Phi = F(r)/r \) little calculation gives

\[
C_2 e^{-\frac{\sqrt{2}}{\lambda_D}} (a + 1) = -\frac{Q}{4\pi \varepsilon_0} \quad \text{and with } a \rightarrow 0 \quad C_2 \rightarrow -\frac{Q}{4\pi \varepsilon_0}
\]
For $a \to \infty$ the potential vanishes as expected and the final solution takes the form

$$\Phi(r) = \Phi_0 e^{-\frac{\sqrt{2}r}{\lambda_D}} \quad \text{with} \quad \Phi_0 = \frac{Q}{4\pi \varepsilon_0} \quad (3.27)$$

Inserting (3.27) this result in form of a Taylor expansion into Equation (3.26) gives

$$\rho(r) = -\frac{Q}{2\pi r \lambda_D^2} e^{-\frac{\sqrt{2}r}{\lambda_D}} \quad (3.28)$$

This result describes the response of a plasma in the vicinity of a positive charge $Q$. The negative sign on the right indicates that a negative space charge is built up around the disturbance. The electrons which are much more mobile than the ions are attracted by the charge and build up a potential barrier. This effect is called Debye shielding since it shields out the disturbing potential exponentially. The classical vacuum potential distribution around a charge which shows the typical $1/r$ decrease is changed to an $\exp(-r)$ form which settles much earlier. At the distance $r = \lambda_D$ the potential is damped down to $\Phi_0/e$. The increased damping is shown in Figure 3.3. It is important to note that for this calculation an expansion has been utilized which requires $e\Phi \ll k_B T$.

**3.3 Floating Potentials**

**3.3.1 Introduction**

Floating potentials are built up on electrically insulated objects in contact with a plasma and are reasoned by current balance. They can reach considerable values depending on
the plasma density. For example during plasma storms after solar flare exhausts potentials on satellites and other spacecraft are reported to reach several thousand volt. The critical point is that parts of the spacecraft that are weakly grounded may observe differential charging due to unequal effective collecting surface areas. This differential charging leads to destruction of sensible electronic devices or sparking. The latter has been observed mostly on solar panels due to their high amount of dielectric surfaces. It is clear that sparking eventually causes serious damage and even fallout of the whole power system due to short circuits.

Payload structures are very susceptible to differential charging too as they are often provided high negative (or positive) voltages in reference to the spacecraft ground. Hence these parts draw overproportional ion (or electron) currents respectively from the plasma. Grounding of payload is a highly sophisticated and important design issue.

Threshold voltages for sparking have been examined for various geometrical configurations and plasma conditions in ground tests in vacuum chambers (see Refs. [18], [19], and references therein). Theoretical assessment has been done by [20], [21], and others.

### 3.3.2 Theory of Floating Potentials

The theory of floating potentials is extracted directly from basic plasma properties such as quasineutrality and movability of the different plasma constituents. Physically the floating potential is defined as the potential difference between an object and the plasma surrounding it. Especially in space one defines the floating potential of a spacecraft as the voltage between the spacecraft surface which in most cases is biased to the spacecraft ground and the ambient plasma. Absolute potentials are referred to the vacuum space potential \( \Phi_0 \) which represents the limit \( \Phi(x) \xrightarrow{x \to \infty} \Phi_0 \).

For exact relation and definition of the potentials appearing on a spacecraft see Figure 4.5. Maxwellian velocity distributions are assumed for ions and electrons, thus the mean velocities \( v_{Th,e} \) and \( v_{Th,i} \) can be calculated using Equation (3.7). Since \( v_{Th} \propto m^{-1/2} \) the electron velocity is much higher than that of the ions. Following [17] one can estimate the ion and electron currents as follows. According to the definition of gas pressure (see Section 3.1.1) \( p = \frac{1}{3} m n \langle v^2 \rangle \) with the mean quadratic velocity \( \langle v^2 \rangle = \frac{3}{2} \frac{k_B T_e}{m} \) the current density can be written as \( j_i = \int_0^\infty dv v p(v) \). Evaluation of the integral yields

\[
j_{i,e} = \frac{e n_{i,e} \langle v \rangle}{4} \tag{3.29}
\]

with indices \( i \) for ions and \( e \) for electrons respectively. Again, since \( m_e \ll m_i \), the electron current must exceed the ion current by far. Thus an initially neutral object brought into contact with plasma receives an effective negative current which charges it negatively until the potential of the object \( \Phi_f \) changes the velocity distributions so that \( \int_A j_e = \int_A j_i \) over the spacecraft surface \( A \). Ions are accelerated causing \( \langle v_i \rangle \) to rise while electrons are decelerated and \( \langle v_e \rangle \) decreases. Hence the local randomized movement of ions and electrons is deformed, resulting in a preferred velocity direction according to the electrical field lines. This effect is closely related to Debye shielding introduced in Section 3.2.1.

The region of modified plasma potential which extends approximately one Debye length from the source of disturbance into the plasma is referred to as the sheath [22]. In order to calculate the absolute change in potential \( \Phi_P - \Phi_f \) equalling \( j_e = j_i \) and assuming Maxwellian velocity distributions in the undisturbed Plasma gives

\[
\Phi_P - \Phi_f = \frac{k_B T_e}{e} \ln \left( \frac{\langle v_e \rangle}{\langle v_i \rangle} \right) \tag{3.30}
\]
The detailed derivation can be found in [17]. This simple model is not complete and needs further discussion which will be continued later on.

Extending (3.29) with the thought that the randomized thermal velocity is given by (3.7), and remembering the density distribution $n_e(x)$ from the Boltzmann relation (3.25) the current density to an object floating in plasma can be expressed as

$$j_e = \frac{e n_0}{4} \left( \frac{8 k_B T_e}{\pi m_e} \right) e^{\frac{|\Phi_P - \Phi_{SC}|}{k_B T_e}}$$

(3.31)

This equation is valid for $\Phi_{SC} < \Phi_P$ which is usually fulfilled. The ion current to the spacecraft is limited to the randomized current approaching the sheath surface from the plasma. Thus the total current density is

$$j = \frac{e n_0}{4} \left( \frac{8 k_B T_i}{\pi m_i} \right) - \frac{e n_0}{4} \left( \frac{8 k_B T_e}{\pi m_e} \right) e^{\frac{|\Phi_P - \Phi_{SC}|}{k_B T_e}}$$

(3.32)

Integrating this density over the entire effective surface of the sheath $A_{Sh}$ gives the total current $I_{SC}$. Focussing on the application of this theory in numerical calculations the total current is added a ram component $I_{RAM}$ caused by the spacecraft flying through ambient plasma. Since in most plasma simulations $\lambda_D \ll L$ with the typical system dimension $L$ the sheath thickness is neglected and integration is conducted over the object surface. This aspect will be discussed later on. For completeness it should be mentioned that several effects result in additional currents which are lower by orders in magnitude compared to the current given by (3.32). These effects are:

- secondary electron emission
  This is shown by [24] to be negligible for the configuration on SMART-1 since bus voltages do not exceed 50 V.

- fast thermal electrons and ions from the sun causing photo emission

- cyclic movement of electrons and ions around small spacecraft parts. This occurs mainly for long cylindrical parts as Langmuir sensors, antennas, … and causes deviations in the classical Debye shielding.

All of these effects are very small and can be neglected. More on the calculation of spacecraft currents in practice is given in the next section 4.3.3.

This simple model is based on the assumption of quasineutrality at the sheath boundaries and the assumption $e \Phi(r) \ll k_B T_e$ which has been introduced for the calculation of Debye shielding in Section 3.2.4. These assumptions cannot be fulfilled in general [23]. If one measures the ion current to an object floating in a plasma of known parameters one finds that this current is much higher by approximately one order in magnitude than the prediction by (3.32). The reason is an oversimplification in the model assuming perfect quasineutrality and equilibrium at the edge of the sheath. In fact at the outer regions of the Debye sphere where $e \Phi$ is equal or below the thermal energy $k_B T$ electrical potential disturbances $\Phi'$ with $e \Phi' \leq k_B T$ can propagate unhindered. These low potentials pre-accelerate ions from far beyond the sheath boundary in direction of the negatively charged object. Arguing this way one gains the right physical picture for the situation.

In order to quantify it one starts by equalling the kinetic energy gained by an ion running down from the plasma to the sheath boundary $x = 0$

$$\frac{m_i v^2(x)}{2} = \frac{m_i v^2(0)}{2} + e[\Phi(0) - \Phi(x)]$$

(3.33)
Assuming collisionless behavior there cannot be ionization or recombination, and hence the current \( e_n(x)v(x) = \text{const.} \). Furthermore at \( x = 0 \) quasineutrality is presumed by stating \( n_i(0) = n_e(0) \). Rearranging gives

\[
n_i(x) = \frac{n_i(0)v(0)}{v(x)} = n_i(0) \left(1 + \frac{2e[\Phi(0) - \Phi(x)]}{m_i v^2(0)}\right)^{-\frac{1}{2}}
\]

Assuming a Boltzmann distribution for \( n_e(x) \) and writing \( e/\varepsilon_0|n_e(x) - n_i(x)| \) at the right side of the Poisson equation as was done in Section 3.2.4 one obtains

\[
\frac{d\Phi(x)}{dx} = \frac{en_e(0)}{\varepsilon_0} \left( e^{-\frac{e[\Phi(x) - \Phi(0)]}{k_B T_e}} - \left(1 - \frac{2e[\Phi(x) - \Phi(0)]}{m_i v^2(0)}\right)^{-\frac{1}{2}} \right)
\]

For a positive space charge (in front of a negatively charged object) then \( \frac{d\Phi(x)}{dx} < 0 \forall x > 0 \). This is called the collector sheath or cathode sheath. The opposite respectively is referred to as the source- or anode sheath. For the first one follows

\[
\left(1 - \frac{2e[\Phi(x) - \Phi(0)]}{m_i v^2(0)}\right)^{-\frac{1}{2}} > e^{-\frac{e[\Phi(x) - \Phi(0)]}{k_B T_e}}
\]

and since for small \( x \) where \( |\Phi(x) - \Phi(0)| < k_B T_e \) (as was derived earlier in this section) the exp can be expanded one gains after rearranging

\[
v(0) > \sqrt{\frac{k_B T_e}{m_i}} \quad (3.34)
\]

This is the Bohm sheath criterium which states that the directed ion kinetic energy at the sheath boundary must be greater than thermal energy. If this is not true the ion density

![Figure 3.4: Potential distribution with presheath taken into account](image-url)
will decrease faster than that of the electrons which leads to a collapse of the sheath. From (3.33) one can determine now the potential at the sheath boundary to $\Phi(0) = k_B T_e / 2e$.

Taking into account these results, and entering the derivation of the floating potential again some corrections to the simple result (3.30) finally lead to

$$\Phi_P - \Phi_f = -\frac{k_B T_e}{2e} \ln \left( \frac{2\pi n_i^2 m_e}{n_e^2 m_i} \right)$$

The detailed derivation can be found in [17] although the ratio of ion and electron densities is omitted there. A similar result can be written for anode sheaths.

In fact these results state that the effective area of an electrically conductive surface faced to a plasma is much greater than the geometrical area. The sheath expands about one Debye length from the object and the presheath even more.

In the derivation above it was assumed that the plasma could maintain arbitrary currents drawn by the object. This is not always true. Since a sheath layer of equal potential is provided its current from layers of ever increasing distance it is clear that the maximum current drawn is limited in time by the maximum available amount of charge in the plasma of each layer. Specializing this to the plasma configuration around SMART-1 one can approximate that the maximum currents of either polarity equal the amount of charge exchange (CEX) ions scattered out of the beam within $\approx 0.5$ m from the thruster exit.

This is the region acting as the main source for CEX ions flowing back to the solar arrays. A very rough estimate for the total amount of the CEX particle flow gives $10^{17} - 10^{18}$ s$^{-1}$. So the maximum currents available for backflow are of the order $10 - 100$ mA. Results of SmartPIC show backflow currents of approximately $1 - 20$ mA for both, electrons and ions. This already represents a serious drain to the plasma. [17] and [25] state independently that the linear sheath theory presented in this chapter is only valid for minor currents drawn from the plasma. For the given backflow current which equals at least 20 % of the total plasma flow the simple theory is definitely outranged and can only be utilized for rough estimates.

The main problem here is that the actual electron number density, and further the electron current is unknown and can only be derived by Boltzmann-type models. Since those calculations break the conservation of charge in assuming an indefinite charge reservoir beyond the sheath they cannot be accurate. Moreover Equation 3.32 had to be evaluated at the sheath boundary. The usual method to integrate over the spacecraft surface introduces an unknown error since in SmartPIC $\lambda_D \approx L$ and the sheath extends far into the CEX plasma. Finding the exact surface of the sheath for integration is not a simple issue due to the plasma being fluctuating and inhomogeneous. An exemplary and approximate curve for the sheath boundary above the solar array is depicted in Figure 3.5. Bearing in mind that the CEX density around the solar array ranges from $10^8$ m$^{-3}$ to $10^{12}$ m$^{-3}$ one can estimate a Debye length of 1 cm to 1 m (see Figure 3.6).
Figure 3.5: Approximate path of the sheath boundary above the solar array (black curve).

Figure 3.6: Debye length range in the vicinity of the solar array

Conservation of charge is the main criteria that has to be taken into account when starting to build an exact model. Since inhomogeneities, complex geometries and potentials cannot be treated analytically the only way to obtain correct values for the backflow currents is a separate self-consistent calculation of ion and electron flows throughout the domain. These thoughts are extended in section 6.7.2.

3.4 Collisions

Collisions between particles in a gas or fluid are stochastic processes. In equilibrium state the frequency and type of collisions is governed by the Brownian thermic movement. If external electromagnetic forces are applied to the system additional collisions due to unequal acceleration of different types of particles have to be considered. The physical field dealing with these effects, providing expressions for calculation of macroscopic parameters, is transport theory.

As discussed in Section 3.1.2 the explicit calculation of the collisional term on the right side of the Boltzmann equation (3.11) is not easy. Following a simplified equation usable in practice will be discussed: The Focker-Planck equation. Attaching on that, some expressions for macroscopic transport parameters will be given.
3.4.1 Hard Sphere Model

For completeness this classical model has to be mentioned here. For the hard sphere model the two particles are seen like billard balls. Their atomic radii $r_1$ and $r_2$ in Figure 3.7 together with the collision parameter $b$ completely define the geometry of the problem. Conservation of impulse and energy give the post-collisional velocities $v_1'$ and $v_2'$. The model is often applied in Monte Carlo simulations.

3.4.2 Coulomb Collisions

As depicted in Figure 3.7 b) the colliding particles do not observe the classical sharp edged trajectories which are typical for “billard” collisions but interact with a potential $U(r)$ depending on the distance $r$ of the particles. Thus the trajectories are smeared out. For small angle Coulomb collisions in a Plasma the effective radius is $\approx \lambda_D$. This can be used to calculate the absolute cross section from

$$\sigma_{tot} = \int_0^{4\pi} \frac{d\sigma}{d\Omega} d\Omega = \int_{b_{min}}^{b_{max}} \int_0^{2\pi} b \, db \, d\varepsilon$$

By restricting to $b_{min} = 0$ and $b_{max} = \lambda_D$ one is able to evaluate the integral. Explicit calculation of the path is cumbersome and uses in a classical point of view elements of variation calculus. In fact at such small sizes quantum mechanics play the dominant role. Thus one mostly prefers a statistical description introduced in the next section.

A more simple approximation can be obtained by using the Rutherford cross section formula

$$\left( \frac{d\sigma_{ij}}{d\Omega} \right)_R = \frac{b_0^2}{4 \sin^4 \left( \frac{\theta}{2} \right)}$$

with $b_0$ being the collision parameter which (according to Section 3.2.1) takes the form

$$b_0 = \frac{Ze^2}{4\pi\varepsilon_0 m_{in} v_{in}^2}$$

where the index $in$ refers to the incident particle.

Figure 3.7: The basic collision models. a) classical hard sphere model. Particles conduct “billard” collisions. b) Coulomb collisions. Particles interacting via an arbitrary potential (in this case Coulomb) observe effective collision cross sections much bigger than the geometrical particle dimensions.
3.4.3 Focker-Planck Equation

Derivation of this equation can be found in most higher level textbooks as [14] or [15]. The essential thoughts will be mentioned shortly here.

Starting at the general Boltzmann collisional term

\[ \left( \frac{\delta f_i}{\delta t} \right)_c = \sum_j \int d\mathbf{v}_j \int \frac{d\sigma_{ij}}{d\Omega} d\Omega (f'_i f'_j - f_i f_j) |\mathbf{v}_i - \mathbf{v}_j| \]  

(3.38)

One starts to replace the differential cross section \( d\sigma_{ij} d\Omega \) by the Rutherford cross section (3.36) and sets \( b_0 \) to the collision parameter for a deflection angle \( \theta = \frac{\pi}{2} \). \( b_0 \) is calculated the same way as in Section 3.2.1 for the collision frequency. The only difference is that instead of using absolute velocities one introduces a differential velocity vector \( \Delta \mathbf{v}_i = \mathbf{v}'_i - \mathbf{v}_i \) which gives the change due to the collision for a particle \( i \). The distribution function \( f(x, \mathbf{v}, t) \) is then expanded into series around the initial particle velocity \( \mathbf{v}_i \). This linearizes the whole collisional term and requires \( \theta < \frac{\pi}{2} \).

Lengthy partial integration of the integrals appearing when collecting all that into (3.38) is only possible by limiting \( b_{\text{max}} \) to the Debye length. The result is the standard form of the Focker Planck equation (FP)

\[ \left( \frac{\delta f_i}{\delta t} \right)_c = \frac{e_i^4}{4\pi \varepsilon_0^2 m_i^2} \ln \Lambda \left[ -\nabla_{\mathbf{v}_i} \cdot (f_i \nabla_{\mathbf{v}_i} H_i) + \frac{1}{2} \nabla^2_{\mathbf{v}_i} : (f_i \nabla^2_{\mathbf{v}_i} G_i) \right] \]  

(3.39)

\[ \text{with } H_i = \sum_j \frac{e_j^2}{e_i^2} \left( \frac{m_i + m_j}{m_j} \right) \int d\mathbf{v}_j \frac{f_j}{|\mathbf{v}_i - \mathbf{v}_j|} \]  

(3.40)

\[ \text{and } G_i = \sum_j \frac{e_j^2}{e_i^2} \int d\mathbf{v}_j f_j |\mathbf{v}_i - \mathbf{v}_j| \]  

(3.41)

\( H_i \) and \( G_i \) are called the Rosenbluth potentials in honor of Marshall N. Rosenbluth (1927–2003). The ‘:\’–operator is defined as \( A : B = A_{ij} B_{ij} \). These expressions obviously are not very useful since the (principally unknown) distribution function still resides on the right side in form of integrals and differential expressions.

The situation gets much simpler if \( f \) is known. Fortunately this is mostly the case for plasmas when one assumes Maxwellian distributions. Coming back once again to the FP equation it can be rewritten to a form showing the physical meaning more intuitively [26]

\[ \left( \frac{\delta f_i}{\delta t} \right)_c = \nabla_{\mathbf{v}} \cdot (\mathbf{D} \cdot \nabla_{\mathbf{v}} f) \]  

(3.42)

where \( \mathbf{D}(\mathbf{v}) \) is a general diffusion coefficient. The form of this equation is the same as that for the continuity equation 3.12 if one replaces the particle flux by the term in parentheses on the right side of Equation (3.42). So the FP equation is simply a continuity equation in velocity space with the flow \( \mathbf{D} \cdot \nabla_{\mathbf{v}} f \). Consequently in this model not single collisions but global particle diffusion due to collisional effects are predicted. This makes the FP equation the ideal basis to start from when treating fluids and other macroscopic systems without strict geometrical ordering under the influence of external forces.

In practice the most important approximation to the FP equation is the Krook friction term already introduced in Section 3.1.2, Equation (3.14). The difficult part left with this is to find expressions for the collision frequency or, more fundamental, the collision cross section. Approximations to that are given in Section 3.2.1 under “Collision frequency”. Review of transport theory is beyond the scope of this work and can be found in most textbooks treating plasmas [26].
3.4.4 Charge Exchange

Besides the collisions changing trajectories of the affected particles in high temperature gasses and plasmas a different kind of collisions exist. In these so called Charge Exchange Collisions (CEX) only electrons are transferred. Collision partners can be ions of different ionization levels or ions and neutrals. The probability for such processes is naturally depending on the ionization level and energy.

Focussing on spacecraft environments CEX particles are mostly generated by collisions between fast ions in the exhaust beam of the thruster with slow neutrals at thermic velocities corresponding to approximately 1000 K. Hence the resulting CEX ions have low kinetic energies and are easily redirected by electric fields. Since the highest production rate of such particles is usually some cm in axial direction from the thruster exit, at the point of the highest plasma density, a great number of CEX ions is repelled by the potential of the beam center (20 – 60 V) which creates a strong radial plasma flow around the beam axis. Details on the flow can be seen in Chapter 6.

Theory on exact calculation of cross sections comes from the field of nuclear physics and is out of the scope of this work.

However experimental data is available in the literature [27], [28], [29] and references therein.
Chapter 4

Physical Model

This chapter gives insight into the practical application of the theory. All relevant constants, evaluation models, constraints, and implementation notes are contained. Before starting with the model description the relevant physical input parameters the simulation is based on should be mentioned. These are collected in Table 4.1.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Sign</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Background neutral density</td>
<td>( n_N )</td>
<td>m(^{-3} )</td>
</tr>
<tr>
<td>neutral density</td>
<td>( n_N )</td>
<td>m(^{-3} )</td>
</tr>
<tr>
<td>ion particle ratio</td>
<td>( P P P_i )</td>
<td>-</td>
</tr>
<tr>
<td>neutral particle ratio</td>
<td>( P P P_n )</td>
<td>-</td>
</tr>
<tr>
<td>ion particle ratio</td>
<td>( P P P_{C E X} )</td>
<td>-</td>
</tr>
<tr>
<td>electron recombination coefficient</td>
<td>( k_4 )</td>
<td>m(^2)K(^{-\frac{3}{2}})</td>
</tr>
<tr>
<td>cross section approximation coefficients</td>
<td>( a )</td>
<td>m(^2)</td>
</tr>
<tr>
<td>cross section approximation coefficients</td>
<td>( b )</td>
<td>m(^2)ln(sm(^{-1}))</td>
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<tr>
<td>elastic collision coefficient</td>
<td>( k_3 )</td>
<td>m(^2)s(^{-1})</td>
</tr>
<tr>
<td>outer insulator radius</td>
<td>( r_o )</td>
<td>m</td>
</tr>
<tr>
<td>inner insulator radius</td>
<td>( r_i )</td>
<td>m</td>
</tr>
<tr>
<td>cathode position relative to emitter center</td>
<td>((x_{cath}, y_{cath}, z_{cath}))</td>
<td>(m,m,m)</td>
</tr>
<tr>
<td>cathode diameter</td>
<td>( d_{cath} )</td>
<td>m</td>
</tr>
<tr>
<td>mass flow rate</td>
<td>( \dot{m} )</td>
<td>ms(^{-1})</td>
</tr>
<tr>
<td>cathode split</td>
<td>( s_{cath} )</td>
<td>%</td>
</tr>
<tr>
<td>ionization efficiency</td>
<td>( \eta_{ion} )</td>
<td>%</td>
</tr>
<tr>
<td>double charged percentage</td>
<td>( \eta_{double} )</td>
<td>%</td>
</tr>
<tr>
<td>ion beam axial temperature</td>
<td>( T_{i,ax} )</td>
<td>eV</td>
</tr>
<tr>
<td>ion beam radial temperature</td>
<td>( T_{i,rad} )</td>
<td>eV</td>
</tr>
<tr>
<td>neutral particle temperature</td>
<td>( T_n )</td>
<td>K</td>
</tr>
<tr>
<td>acceleration voltage</td>
<td>( U_{acc} )</td>
<td>V</td>
</tr>
<tr>
<td>emitter reference potential</td>
<td>( \Phi_{ref} )</td>
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</tr>
<tr>
<td>inner beam divergence angle</td>
<td>( \alpha_i )</td>
<td>rad</td>
</tr>
<tr>
<td>outer beam divergence angle</td>
<td>( \alpha_o )</td>
<td>rad</td>
</tr>
<tr>
<td>far field electron temperature</td>
<td>( T_{e\infty} )</td>
<td>eV</td>
</tr>
<tr>
<td>adiabatic coefficient</td>
<td>( \gamma )</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4.1: Physical input parameters for the simulation
4.1 Ions and Neutrals

Atomic sized particles are treated as so called *super particles*. One computer particle represents a great number of physical particles, thus, radically decreasing the computational effort. This method is widely used in particle-in-cell (PIC) simulations (Section 5.1.5). For densities of approximately $10^{15}$ m$^{-3}$ it is simply not possible to treat single physical particles. Thus one has to compromise very little physical inaccuracy to feasibility of the whole calculation. In SmartPIC particle rations of $10^8 \sim 10^{10}$ m$^{-3}$ particles per super particle are used. In that way the overall number of particles in the simulation does not exceed $10^6$ which is feasible on a standard workstation PC.

4.1.1 Velocity Distribution and Initialization

New particles are introduced to the simulation at the thruster exit and the neutralizer. Geometrical definitions can be seen in Figure 4.1. Description of the initializing procedure is given subsequently.

![Figure 4.1: Geometry of the beam at the thruster exit. Inner and outer divergence angles define the beam formation.](image)

**Ions**

The amount of ions to be inserted in a time step $\Delta t$ is derived from the emitter ion current $I_{ie}$ by

$$
\Delta n_i = \frac{I_{ie}}{PPF_i} \Delta t \quad \text{and} \quad I_{ie} = \frac{\dot{m}(1 - s_{cath})\eta_{ion}}{m_i(1 + \eta_{double}V/2)}
$$

(4.1)
In accordance to the Hall thruster function principle (Section 2.5.1) ions are inserted at a velocity
\[ v_i = \sqrt{\frac{2eU_{\text{acc}}}{m_i}} \]  
(4.2)
with \( U_{\text{acc}} \) being the thruster's acceleration voltage between anode and cathode which, in case of the PPS-1350, is 350 V. Doubly charged ions respectively acquire a velocity higher by a factor \( \sqrt{2} \) due to the higher charge. The uniform velocity distribution can be seen in outputs of the virtual RPA measurements in Section 6.2 where it causes small peak widths. This might be subject to criticism because in a real Hall thruster the point of ionization, and hence the kinetic ion energy, varies for each injected ion. Thus the effective acceleration voltage is different for every ion. In fact a Gaussian distribution around some velocity \( \langle v_i \rangle \) would be more correct. This is one of the items on the task list for future versions of the simulation. However the uniform distribution, to the current level of understanding, did not introduce great errors.

The initial position of an ion is given by its radius \( r \) taken to be uniformly distributed between \( r_i < r < r_o \), the angle \( \alpha_\Theta \), taken to be uniformly between \( 0 < \alpha_\Theta < \pi \) and the \( z \)-coordinate which is determined by the height of the thruster exit \( z_{\text{Thruster}} \). The cartesian coordinates used for insertion are then calculated by
\[ x_i = r \cos(\alpha_\Theta) \]
\[ y_i = r \sin(\alpha_\Theta) \]
\[ z_i = z_{\text{Thruster}} \]
The direction of the velocity \( v_i \) is determined in spherical coordinates \( (v_i, \alpha_1, \alpha_2) \). Determination of \( \alpha_1 \) is done by randomizing between \( 0 \leq \alpha_1 < 2\pi \). \( \alpha_2 \) is varied in accordance to the radial position by
\[ \alpha_2 = \frac{\alpha_i - \alpha_o}{r_o - r_i} (r - r_i) + r_i \]
In addition, a stochastic thermal component is added to this geometrically exact distribution. It consists of an axial, and a radial component, both determined by a Boltzmann distribution parametrized by axial and radial temperatures \( T_{i,ax} \) and \( T_{i,rad} \) respectively. The \( \alpha_{1,Th} \) component is randomized between \( 0 < \alpha_{1,Th} < 2\pi \). Finally the according cartesian velocity components are computed as
\[ v_{i,x} = v_i \sin(\alpha_2) \cos(\alpha_1) + v_{Th,rad} \cos(\alpha_{1,Th}) \]
\[ v_{i,y} = v_i \sin(\alpha_2) \sin(\alpha_1) + v_{Th,rad} \sin(\alpha_{1,Th}) \]
\[ v_{i,z} = v_i \cos(\alpha_2) + v_{Th,ax} \]
with the axial and radial thermal velocities \( v_{Th,ax} \), and \( v_{Th,rad} \) respectively.

**Neutrals**

The PPS-1350 uses a hollow cathode type that is flown through by neutral propellant. The fraction of the total mass flow is approximately 8% and is represented by \( s_{\text{cath}} \) in the simulation.

The amount of neutrals per time step expelled by the emitter is given by
\[ \Delta n_{n,em} = \frac{I_{mn,em}}{PPP_n} \Delta t \quad \text{and} \quad I_{mn,em} = \dot{m} (1 - s_{\text{cath}}) \frac{1}{m_n} (1 - \eta_{\text{ion}}) \]
Accordingly the following relation yields the number of neutral super particles to be inserted at the cathode

\[ \Delta n_{\text{cath}} = \frac{I_{\text{mn,cath}}}{P P P_n} \Delta t \quad \text{and} \quad I_{\text{mn,cath}} = \frac{\dot{n}_{\text{s,cath}}}{m_n} \]

For both entry points the spatial distribution is uniform over the cathode exit area. The procedure is similar to that for ions. Since neutrals are not affected by the electric field the velocity is defined by a Boltzmann distribution parametrized by the mean neutral temperature \( T_n \). Vector alignment is done by assuming a uniform distribution \( 0 < \alpha_1 < 2\pi \) for the tangential component and a uniform distribution \( -\frac{\pi}{2} < \alpha_2 < \frac{\pi}{2} \) for the vertical ratio. Cartesian velocities are obtained similar to the thermal component for ion velocities given in the preceding section.

### 4.1.2 Movement

Movement of the particles in general is done by a leap frog scheme (Section 5.1.6). Such is widely utilized due to a reduced error and higher accuracy in PIC simulations. It is fully included in this simulation. Velocities are first calculated for half a timestep based on the fields. In advance particles are moved and particle velocities are set to their final values for a full time step.

Ions are governed by the equation

\[ x_i(t + \Delta t) = x_i(t) + \left( v_i(t) + \frac{E_i}{2m_i} \right) \Delta t \quad (4.3) \]

which is conformal with the leap frog algorithm. Neutrals move at constant thermal speed, being redirected only by collisions.

\[ x_n(t + \Delta t) = x_n(t) + v_n(t) \Delta t \quad (4.4) \]

Special treatment in terms of nonlinear velocity flow effects and gas pressure forces is applied only for electrons in the advanced electron fluid model (Section 4.5). If a particle traverses one of the outer domain boundaries (see Figure 5.8) it is removed from the simulation and accounted for thrust measurements. The only exception in this case is the -Y boundary plane at which particles are reflected due to symmetry (see Section 4.3.1). If a particle hits the spacecraft surface it is accounted for backflow current calculation if the surface hit is conducting, or just removed from the simulation in the case of a non-conductive surface. If a particle is redirected into the thruster cavity it is re-ejected in the next time step.

### 4.1.3 Time Steps

According to the Sampling Theorem known in measurement theory (also taken as stability criteria for the leapfrog scheme) the minimal frequency \( \nu_{s,\text{min}} \) to resolve data with eigen-frequency \( \nu_0 \) is given by \( \nu_{s,\text{min}} \leq \nu_0 \). Since no gyration movements or plasma waves are included in this simulation the only element left to define a criteria for time steps is the movement of ions. Hence one can state that

\[ \Delta t_{\text{max}} = \frac{1}{2} \frac{\Delta x_{\text{min}}}{v_p} \]
where \( v_p \) is the velocity of particle \( p \). As discussed in Section 4.1.1 it can be determined by 
\[
\v_p = \sqrt{\frac{2U_{acc}m_p}{e}}.
\]
The highest velocities should be acquired by double charged ions with charge \( e_{\text{double}} = 2e \). The requirement then is 
\[
\Delta t_{\text{max}} = \Delta x_{\text{min}} \frac{m}{4 \sqrt{U_{\text{acc}} e}}
\]

(4.5)
The maximum speed for \( \text{Xe}^{2+} \) and \( U_{\text{acc}} = 350 \text{ V} \) is \( 3.1197 \times 10^4 \text{ ms}^{-1} \) which is by far more than the 354 ms\(^{-1} \) thermal speed at 1000 K. Hence the Numerical Heating Criterion used by [8] which takes the thermic movement of neutrals as a reference is fulfilled automatically.

In order to reduce the computational effort only the finest grid level 5 is computed at every level. Since grid sizes are related by a factor 2 from one level to the next, and the time steps exhibit the same behavior, level \( M \) has to be computed only at every \( 2^{5-M} \)th time step. The scheme can be depicted as in Figure 4.2. The resulting time step sizes are collected in Table 4.2. For further information on the grid and the level structure please refer to Section 5.2.2.

The error introduced by this multiple time stepping scheme is kept down by ensuring an overlap between the boarders of grid domains of different level. If two or more boundaries coincide spatially ions approaching from the fine grid region would form a crowd until the coarse grid is processed. This would lead to continuous “ripples” in the density distribution. In fact such an effect has not been observed. Hence the error is assumed to be negligible.
4.2 Collisions

The collision model has been left unchanged, taken from previous versions of SmartPIC. A complete description of the model can be found in [30].

The general scheme is the same for all collision types considered. First a probability

\[
\begin{align*}
Xe^+ + Xe & \xrightarrow{\text{elastic}} Xe^+ + Xe \\
Xe^{2+} + Xe & \xrightarrow{\text{elastic}} Xe^{2+} + Xe \\
Xe^+ + Xe & \xrightarrow{\text{CEX}} Xe + Xe^+ \\
Xe^{2+} + Xe & \xrightarrow{\text{CEX}} Xe + Xe^{2+} \\
Xe^{2+} + Xe^+ & \xrightarrow{\text{CEX}} Xe^+ + Xe^{2+} \\
Xe^{2+} + e^- & \xrightarrow{\text{recomb.}} Xe^+ \\
Xe^{2+} + e^- & \xrightarrow{\text{recomb.}} Xe^+
\end{align*}
\]

Table 4.3: Types of collisions implemented in the current version

\[P(i, j)\] for the current interaction between particles \(i\) and \(j\) is calculated. This probability is compared with a randomized number \(n_r\) with \(n \in [0..1]\). If \(P > n_r\), the collision takes place and the relevant changes are computed by the code.

4.2.1 Ion Ion Collisions

Since collision frequencies strongly depend on temperature and density, and show highly nonlinear behavior the usual approach is to fit experimental curves by polynomials of high degree. Such methods are reviewed in [8]. For determination of the exact cross sections a simple approximative formula has been derived in [27] which is widely used in most PIC simulations currently under development

\[
\sigma_{\text{CEX}}(\Delta v) = (k_1 \ln \Delta v + k_2)^2 \quad (4.6)
\]

\(\Delta v\) is the impact velocity in [ms\(^{-1}\)]. Values for the constants \(k_1\) and \(k_2\) can be derived by evaluation of the exact form of (4.6) found in [27]. The resulting cross sections have been compared by [8] to experimentally obtained results found in [29]. It has been found that the theoretical predictions are approximately 20% below the experimental values. Previous versions of SmartPIC implemented this model successfully. However, in more recent measurements [29] and theoretical assessments [28] it has been shown that the results of [27] are definitely too low. Another slightly changed model is preferred:

\[
\sigma_{\text{CEX}}(\Delta v) = a - b \ln \Delta v \quad (4.7)
\]

A comparison of the two models and experimental data by [29] has been conducted in Figure 4.3 and the model (4.7) shows definitely better functional and absolute fitting. Thus in the current simulations this model is applied.

The probability \(P\) for a CEX collision of two ions of different ionization level with relative velocity \(\Delta v\) over a time step \(\Delta t\) can be calculated with a standard relation used in Monte Carlo schemes.

\[
P(\Delta v) = 1 - e^{-\Delta v \sigma_{\text{CEX}}(\Delta v) \Delta t} \quad (4.8)
\]

If the exchange takes place the ion is turned into a neutral and vice versa.
Figure 4.3: Comparison of CEX cross section models for $\text{Xe}^+ + \text{Xe} \rightarrow \text{Xe} + \text{Xe}^+$ CEX collision.

Table 4.4: Constants for the model (4.6) based on the theory of [27].

<table>
<thead>
<tr>
<th>Collision</th>
<th>$a$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Xe}^+ + \text{Xe} \rightarrow \text{Xe} + \text{Xe}^+$</td>
<td>$1.71 \times 10^{-18}$</td>
<td>$1.18 \times 10^{-19}$</td>
</tr>
<tr>
<td>$\text{Xe}^{2+} + \text{Xe} \rightarrow \text{Xe} + \text{Xe}^{2+}$</td>
<td>$1.03 \times 10^{-18}$</td>
<td>$7.70 \times 10^{-20}$</td>
</tr>
<tr>
<td>$\text{Xe}^{2+} + \text{Xe}^+ \rightarrow \text{Xe}^+ + \text{Xe}^{2+}$</td>
<td>$4.32 \times 10^{-19}$</td>
<td>$2.8 \times 10^{-20}$</td>
</tr>
</tbody>
</table>

4.2.2 Ion Neutral Collisions

For calculation of the CEX cross section the same method as for ion–ion CEX collisions is utilized (4.6).

Elastic collisions are calculated by a simple model introduced by [31]:

$$\sigma_{el} = \frac{k_3}{\Delta v}$$ (4.9)

With the constant $k_3$ given by [32] as $6.42 \times 10^{-16}$ for $\text{Xe}^+ + \text{Xe}$, and $1.28 \times 10^{-15}$ for $\text{Xe}^{2+} + \text{Xe}$. The probability then takes the form

$$P(\Delta v) = 1 - e^{-\Delta v \sigma_{CEX n n} \Delta t}$$ (4.10)

where the neutral speed $v_n$ is neglected for the calculation of $\Delta v$ due to $v_n \ll v_i$.

4.2.3 Electron Ion Collisions

Electrons do not collide with ions but recombine with them to neutral particles. The probability for such an event can be evaluated using

$$\sigma_{re} = k_4 \sqrt{T_e}$$ (4.11)

where the constant $k_4$ is given by [33] to $2.0 \times 10^{-18}$.
4.3 Potential Calculations

The electric potential Φ is a critical factor in the simulation of ion backflow. It is generated by two sources: the plasma itself, and potentials on the surface of the spacecraft. Both are likely to fluctuate. CEX ions are mainly directed by the electrical fields derived from the potential solution. Thus it is necessary to update the fields instantly with potential variations of the spacecraft and the plasma. In SmartPIC the total solution is acquired by superposition of a pure Poisson distribution based on the potentials emerging from the spacecraft, and a solution for the plasma potential based on the Boltzmann relation (3.25).

4.3.1 Spacecraft Potentials and Boundary Conditions

Since the potential distribution on the satellite is highly complex, especially at the solar array, it is necessary to provide an appropriate spatial resolution. This is guaranteed by the multigrid with resolution \( \Delta x = 8.594 \times 10^{-3} \text{m} \). Interconnector structures and potential distributions on the surface of the solar array can be resolved accurately. According to the definitions in Section 2.2 the potentials on the solar array are set along solar cell strings. Interconnectors are set to the potential of the cells they connect. In order to simulate secondary electron emission a so called shielding factor \( \eta_{\text{Sh}} \) has been introduced. It is shown in Ref. [34] that secondary emission is responsible for a complete shielding of electric potentials underneath a dielectric surface. Irregular variations of the surface potential appear only on the edges of junctions metal ↔ dielectric. The spatial extent of these boundary zones is much smaller than the finest grid size of 8.59 mm in SmartPIC. Hence perfect planar shielding is assumed. \( \eta_{\text{Sh}} = 100\% \) means total shielding which corresponds to a viewable surface potential of 0 V. In the simulation factors \( 70\% < \eta_{\text{Sh}} < 90\% \) have been used. Despite the results of [34] show no effective shielding on Interconnectors in SmartPIC better results are obtained with little shielding \( \eta_{\text{sh,IC}} \approx 20\% \) for the Interconnectors. For details please refer to Chapter 6. Figure 4.4 shows the potential distribution for one representative solar panel. The spacecraft ground is initially set to 0 V. It is continuously updated and set to the calculated floating potential.

Remark: Updation of the spacecraft ground is an optional feature in the simulation that has not been utilized for all runs. Details on the influence of updating can be found in Chapter 6.

The computational domain is set up to include one half of SMART–1 (see Section 5.2 for details on the domain and grid). At the -Y boundary which represents the symmetry plane particles are reflected. All other domain boundaries are permeable. At each boundary of the computational domain a Von Neumann (see Section 5.1.1) condition states that \( \nabla_n f_{ijk} = 0 \) for each function or field \( f \) and the boundary surface normal vector \( n \) pointing outwards. In other words domain boundaries act like mirrors. This is very useful at the Y-plane where all field solutions require mirroring. On the other hand this feature is the main reason for non-convergence of the multigrid solver. When solving for the electric potential, iterating long enough, the solution converges like there was another satellite at equal distance to every boarder (Section 5.4). However these problems do not represent a major treat.

Spacecraft surfaces are provided a Dirichlet boundary condition for the electric potential. They are assigned to a potential according to their position. Potential settings are collected
Figure 4.4: Static potential distribution of the solar array at an exemplary $\eta_{Sh} = 50\%$. Interconnectors range from 0–50 V while glass surfaces are respectively set to 0–25 V.

During a simulation run the surface potentials are optionally updated continuously by the floating potential according to the dependencies depicted in Figures 4.5 and 2.5.

<table>
<thead>
<tr>
<th>Surface type</th>
<th>Potential [V]</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>conductive to ground</td>
<td>$-2$</td>
<td></td>
</tr>
<tr>
<td>thruster ceramic parts</td>
<td>0</td>
<td></td>
</tr>
<tr>
<td>thruster cavity</td>
<td>$\Phi_{ref}$</td>
<td>input parameter</td>
</tr>
<tr>
<td>solar cells (glass)</td>
<td>0-50</td>
<td>depending on $\eta_{Sh}$, input parameter</td>
</tr>
<tr>
<td>interconnectors</td>
<td>0-50</td>
<td>according to position</td>
</tr>
</tbody>
</table>

Table 4.5: Surface potential settings
Figure 4.5: Spacecraft potential scheme. All absolute potentials are referred to $\Phi_\infty$. Spacecraft, and plasma are floating. The thruster exit itself is insulated from the spacecraft.

### 4.3.2 Plasma Potential

The plasma potential is obtained by simply applying the Boltzmann relation (3.25) at every grid point with non-vanishing ion density. This model assumes quasineutrality which is a reasonable presumption for the plume region. At greater distances in the CEX regime the assumption is broken due to the fields emerging the solar array. This is the motivation to find an alternate model which will be discussed further in Section 4.5.

For the current implementation the reference potential $\Phi_0$ is taken at the thruster exit and evaluates to $\Phi_{SC} + 18$ V. The reference electron density itself is calculated via the Boltzmann relation setting $n_e,0 = n_i,0$.

\[
  n_e,0 = n_{i,exit} e^{k_B \left[ \frac{e \Phi_0}{T_e,0 n_{i,exit}^{\gamma} n_{\text{norm}}} \right]},
\]

with the neutralizer density normalization constant $n_{\text{norm}}$ and the adiabatic exponent $\gamma$ used for electron temperature calculation. The temperature correction is due to the variable model presented in Section 4.4.

**Remark:** Principally the plasma potential could be solved together with the spacecraft-based potentials by taking an expression $(e/\varepsilon_0) [n_i - n_e]$ with $n_e$ being obtained by the Boltzmann relation. However this would take several iterations over the calculation of $T_e$, $n_e$, and $\Phi$ which further caused a drastic rise in computational times. Since the plasma densities in regions of noteworthy potential propagation are very low $< 10^{12}$ m$^{-3}$ the deviation from a Coulomb potential is minor. In addition in overlap regions of spacecraft potentials and plasma potentials the latter ones are higher by at least one order of magnitude. Hence the error induced by simply superimposing the two potential solutions is found to be negligible. In the proposed advanced electron model (Section 4.5) the absolute charge densities will be known and allow for physically correct and accurate solution.
4.3.3 Calculation of Floating Potentials

The model for calculation of floating potentials in previous versions relies on the simple model presented in section 3.3.2. The basic idea is to derive the value for the potential from current conservation. Recently [35] wrote the current balance as

\[ I_i = I_{th} + I_r + I_B + I_E \]  

(4.13)

with the total spacecraft ion current \( I_i \), the thermal current \( I_{th} \) which equals the contribution of the first term in Equation (3.32), the ram component \( I_{RAM} \), the CEX ion backflow \( I_B \), and the exhaust current of the thruster \( I_E \). The CEX ion current \( I_{CEX} \) is easily determined by counting CEX ions colliding with surfaces in each time step. \( I_E \) is obtained from counting ions at the thruster exit and the other currents are calculated analytically. Totalling this one can state that

\[ I_i = \frac{e n_{i0} A_{SC}}{4} \sqrt{\frac{8 k_B T_i}{\pi m_i}} + e n_{e0} v_{SC} A_{RAM} + I_B + I_E \]  

(4.14)

with the spacecraft velocity \( v_{SC} \) and the effective ram area \( A_{RAM} \). Thermal equilibrium assures \( T_e = T_i \). Assuming a negatively charged spacecraft the electron current can be derived by extending (3.31) by the contribution of electrons pulled to the spacecraft by CEX ions, the neutralizer electron current \( I_N \) and the additional electron current to the interconnectors, \( I_{INT} \).

\[ I_e = -\frac{e n_{i0} A_{SC}}{4} \sqrt{\frac{8 k_B T_i}{\pi m_e}} e^{\frac{\Phi_{SC} - \Phi_{P}}{k_B T_i}} - \int d\mathbf{f} \left[ \frac{e n_{CEX} A_{SC}}{4} \sqrt{\frac{8 k_B T_{CEX}}{\pi m_e}} e^{\frac{\Phi_{SC} - \Phi_{CEX}}{k_B T_{CEX}}}} \right] - I_N - I_{INT} \]  

(4.15)

For \( n_{e0} \equiv n_{i0} \equiv n_0 \) the reference density of \( 10^{12} \text{m}^{-3} \) is taken into account. \( T_{e0} \) is assumed to be 0.1 eV and \( \Phi_{CEX} \) is set to the local plasma potential. The spacecraft floating potential then can be calculated equalling \( I_e = I_i \). Due to the surface integral this expression cannot be solved analytically as with Equation (3.30) or even the more complex model used by [25]. The problem has to be evaluated numerically instead. Therefore an iterative algorithm is utilized which varies an initial assumption for the potential, calculates the total currents based on this parameter, and adapts the assumption to converge to a minimum difference \( |I_e| - |I_i| \).

Recent results are quite satisfactory despite the questionable assumptions of quasineutrality and the limitations due to linearity in the sheath model underlying this calculation. For accurate and reliable calculation of the spacecraft floating potentials one has to rebuild the model without relying on doubtful assumptions. The aim is to find a self-consistent solution for both, electron and ion density distributions. This is the motivation for the development of a more sophisticated model which allows for \( n_e \neq n_i \). Discussion on this aspect will be continued subsequently in the next chapter 4.5.

4.4 Electron Temperature

The electron temperature is evaluated using the adiabatic energy equation in its non-differentiated form

\[ k_B T_e n_e^{\gamma+1} = C_1 \]

where \( \gamma = 1.28 \) and \( C_1 = 8.76 \times 10^{-5} \) are derived from experimental results (see [32] and references therein).
4.5 Advanced Electron Fluid Model

This section presents the current electron model as well as an experimental model that will be used in future versions of SmartPIC. Starting at the simple quasineutral model historically used in this simulation as well as most other PIC computations (for example [11], [12], [25]) a review of the physical and computational aspects of the electron description and accompanying subjects is given. Finally advanced approaches currently under development are presented.

4.5.1 Fluid Model previously utilized in SmartPIC

In previous versions of SmartPIC quasineutrality \( n_e = n_i \) has been assumed. Thus for all effects depending on the electron density substitution to the ion density reveals correct results. Two physical quantities have been calculated based on this assumption: plasma potential and electron temperature.

The plasma potential can be computed via the Boltzmann relation (3.25) which takes the form

\[
\Phi_P = \frac{k_B T_e(x)}{e} \ln \left( \frac{n_e}{n_{e0}} \right)
\]

(4.16)

The electron temperature in this model is obtained using the adiabatic energy equation (3.2.3) already presented in the preceding section.

A critical remark: Throughout the simulation the emitter exit is taken as reference point. Hence the reference potential \( \Phi_0 = 0 \) is omitted in (4.16) when calculating plasma potentials. The spacecraft ground \( \Phi_{SC} \) is assumed to be at 0 V; potentials propagating from the solar array into space are relative to \( \Phi_{SC} \). It is important to note that the potential scheme depicted in Figure 4.6 in contrast to the new scheme in Figure 4.5 the emitter exit is not electrically insulated and therefore has to refer to the spacecraft ground. This method seems to be questionable due to inconsistency. Since a vacuum potential \( \Phi_\infty = 0 \) V is assumed throughout the simulation and potential gradients emerging from the solar array are solved to converge to \( \Phi_\infty \) the solution \( E = -\nabla \Phi \) is only correct if the spacecraft is permanently biased to the vacuum potential. But floating potentials \( \Phi_f \) would change spacecraft potential to \( \Phi_{SC} = \Phi_\infty + \Phi_f \) and, thus, the electric field configuration had to be different. Furthermore \( \Phi_{ref} \) had to be attached to the floating potential by \( \Phi_{ref} = \Phi_{SC} + 18 \) V. None of these facts are considered.

If, on the other hand, potentials are always referenced to the emitter exit, spacecraft potential would have to be set to \( \Phi_{SC} = -\Phi_{ref} = -18 \) V and vacuum had to be at \( \Phi_\infty = -\Phi_{ref} - \Phi_f \). This is considered neither.

CEX particle movements are governed by the field gradients. When being pushed out of the plume into the region of dominant solar array potentials they observe a potential too high by \( \Phi_{ref} = 18 \) V, the not accounted potential difference \( \Phi_{ref} - \Phi_{SC} \).

However in the current version all potentials are consistently referenced to \( \Phi_\infty = 0 \) V (see Figure 4.5 and Section 4.3.1). Optionally the spacecraft ground is updated with the floating potential.
Figure 4.6: Potential distribution in previous versions of SmartPIC. All potentials are referenced to spacecraft ground but the plasma potential which references to the emitter exit voltage \( \Phi_{\text{ref}} \). The spacecraft ground is biased to \( \Phi_{\infty} \).

4.5.2 General considerations

When searching for an alternative for the quasineutrality assumption one has to be careful to find a solution that is both, physically correct and computable in reasonable times. Somehow motion of electrons must be determined in a consistent way balancing binding to the ions and following potential gradients impinging the plasma. Some general considerations have to be prepared before going into detail.

Time consistency and principal approaches for particle treatment

Since ions and neutrals are treated as kinetic particles their movement is completely defined by the Lorentz force, collisions, and initial conditions. The time base in the simulation is therefore bound to the mass of the lightest particle in order to fulfill the consistency condition that a particle must not travel more than one grid cell in one time step (See Section 4.1.3. This means

\[
\Delta t_{\text{max}} \leq \frac{\Delta x}{v_{\text{max}}} \tag{4.17}
\]

where \( \Delta t_{\text{max}} \) is the greatest acceptable time step in a grid with spacing \( \Delta x \) and particles travelling at speeds \( v < v_{\text{max}} \). The maximum speeds are limited by the inertia of the particles when being accelerated by fields. Thus one can state that the time to cross a distance \( \Delta x \) for electrons and ions being accelerated by the same force \( F \) can be expressed as \( \sqrt{2\Delta x m_{i,e}/F} \). Following the ratio of time bases fulfilling the requirement (4.17) for Xe is

\[
\frac{\Delta t_i}{\Delta t_e} = \sqrt{\frac{m_i}{m_e}} = 491.3255
\]

It is clear that taking electrons into account as kinetic particles results in an enormous increase in computational time and, thus, is not feasible.
Two approaches exist to cope with this problem. The first one treats electrons as virtually heavier particles (also done successfully by [8]). Thus the ratio of time bases is decreased to a level that can be computed in reasonable time. One refers to this approach as the **Heavy electron approach**. This technique of course brings the disadvantage of loosing temporal effects with short characteristic time constants such as the electron cyclotron movement. In practice those high frequency effects are only taken into account if domains of small extent and high spatial resolution are used, for example the simulation of secondary electron emission from a small piece of material. In that case one has to treat a relatively small amount of particles and, thus, can omit the heavy particle approach using the real masses of the electrons and operating with very little time steps far below 1ns. When computing large domains such as the exhaust of an ion thruster or a fusion reactor enormous amounts of particles have to be simulated. The influence of a single particle can be neglected and typical characteristic times are \( \gg 1 \mu s \). If electrons are to be treated as particles it is advisable to compact a large number of them into one representative super electron as is done for the particle in cell method (see Section 5.1.5) and equip them with appropriate higher mass.

The second approach is to treat the ion distribution as boundary condition for an electron fluid. The electrons are not treated as discrete kinetic particles but as a massless fluid. A steady solution for the electron distribution is sought. The fluid point of view again kills high frequency effects but inherently brings some advantages. Collisions don’t have to be treated specially but are included in form of the pressure tensor and the substantial derivation. See Section 3.1.2 for details. This method is referred to as the **electron fluid approach**. In practice fluid models are applied whenever great domain sizes and a huge amount of particles is to be simulated, and single particle interactions are not relevant for calculations. Thus a statistical view of the physical situation is preferred.

**Debye length and sheath conditions - continued**

Resuming the discussion in Section 3.3.2 the standard Boltzmann scheme to obtain electron densities cannot be applied – at least in the vicinity of the solar array. In addition to the problems already mentioned the solar array’s potential distribution introduces additional complexity. Not only negatively biased surfaces appear, as assumed for the derivation in Section 3.3.2, but also such at high positive potentials. Interconnectors placed side by side with structures biased to spacecraft ground build up complicated potentials propagating into the plasma. In fact it is completely unknown if, and how sheaths form for such configurations.

This whole discussion is only intended to show that the analytic models based on classic sheath theory by Langmuir cannot give reliable results for the floating potentials on SMART–1. The same has to be stated for the electron density solution obtained by the Boltzmann relation.

As mentioned before an essential need for a physically correct calculation is to obtain a self-consistent solution for the electron density with the ion distribution as boundary condition. Coupling is automatically given by electric fields. Conservation of charge, momentum, and mass have to be respected.

Based on these requirements the total backflow to the spacecraft can then be easily and accurately evaluated.
Thresholds of the PIC method

In the near field of the plume high densities of $10^{14} - 10^{17}$ m$^{-3}$ require high spatial resolution according to the Debye length which takes values $2 \times 10^{-3} - 8 \times 10^{-5}$ m respectively. The chosen minimal grid size of 8.59375 mm is well above this Debye length. However, due to the strongly directed initial velocity of the ions only small variations in the flow may occur in those regions of high density. Therefore the error arising from relatively coarse resolution in both, time and space, should vanish. On the other hand the high resolution introduces major problems in calculating the potential from given charge distributions by the multigrid solver (Section 5.3.5). To understand this one has to review the PIC concept (Section 5.1.5). Densities on the grid points are set by linear interpolation of the particle numbers according to their position in a grid cell. The number density $n_{ijk}$ at a specific point $(i,j,k)$ is calculated by

$$n_{ijk} = \sum_{p=1}^{N} PPP_p f_{p,ijk} \left(\Delta x\right)^3$$

(4.18)

where $PPP_p$ is the super-particle to physical particle ratio for a computational particle $p$, $f_{p,ijk}$ is the interpolation factor to the point at position $(i,j,k)$, $\Delta x$ is the grid spacing, and $N$ is the number of computer particles in the grid cell. At this point the physical meaning of density has to be rethought critically. A density is a statistical representative value of the number of countable instances of a physical property per unit space volume. In the case of a number- or charge density it represents the mean number of particles or charges per unit volume. This definition requires $N \gg 1$. If one takes into account densities of $n_i \approx 10^{17}$ the PIC method results for a super-particle to real particle ratio of $8 \times 10^9$ on the finest grid level with $\Delta x = 8.59375 \times 10^{-3}$ m in only 7.93 particles per grid cell. Thinking further it is obvious that for $\Delta x \to 0 : n_i \to \infty$. For the region near the thruster exit this means that locally great variations in the density appear. The amplitude of this discrete noise is higher by orders than for example thermal fluctuations, and leads to very high local potential gradients further causing indeterministic ion accelerations and diffusion. This is the main source of instability for any kinetic treatment of electrons.

Two possible solutions offer to solve the problem. At first the super-particle per particle ratio could be reduced. Since some parts of the simulation feature an $O(N^3)$ behavior in the overall number of particles this causes dramatic increase in computational time. Tests have shown that a reduction of the ratio from $8 \times 10^9$ to $5 \times 10^8$ increases the computational time by a factor 3. The second approach is to smooth the resulting densities on the finest grid levels. On the first thought this is a loss in detail information but the use of coarse particle resolutions (PPP ratios) eliminates the details by the discrete noise anyway.

Grid resolution

As discussed in the previous section the grid resolution should be as fine as possible to adapt to the Debye length, at least in the plume. On the other hand it is not feasible to fill the whole computational domain with this fine grid. For example for the $2 \times 7.5 \times 2$ m$^3$ computational domain $4.73 \times 10^7$ gridpoints would require over 15 GB computer memory. This is simply not feasible, at least on available PC workstations. Thus one has to restrict the high resolution to well selected, bounded domains in regions such as the solar array or the thruster exit. See Section 5.2 for details.
Generally in SmartPIC the problem is that on the one hand high spatial resolution and single particle interactions, at least for ions and neutrals, are required and on the other hand a huge spatial domain has to be computed. This combination rules out most of the methods usually applied for plasma simulations.

**Estimation of beam parameters**

Previous simulations have shown that the ion densities range from about $10^{17} \text{m}^{-3}$ close to the emitter exit down to $10^8 - 10^{12} \text{m}^{-3}$ in the far field region. That is quite a wide range and different effects are dominating the plasma behavior at each end of the scale. Debye lengths range from 8 $\mu$m up to half a meter. Electron temperatures have been measured in ground tests of the thruster confirming the results of simulations. In the far field temperatures are mostly constant at 0.6 eV while the exhaust plume exhibits temperatures up to 10 eV with high gradients according to the density distribution. Adiabatic behavior can be expected due to the relatively low density (compared to $10^{20} - 10^{23} \text{m}^{-3}$ in Arcjet or magnetoplasmodynamic thrusters) and low particle interaction rates. This is a widely used assumption used even in kinetic models.

The plasma can be assumed as non-collisional because in the region of highest density and temperature the following relation holds $\omega_{pe} \approx 1.78 \times 10^{10} \text{s}^{-1} \gg \nu_{ei} \approx 1.33 \times 10^5 \text{s}^{-1}$.

External fields are assumed to be purely electrostatic but exhibit high gradients in regions of density fluctuations and in the near field of thruster and solar array where the simulation has shown values up to 5,000 V/m. This in advance influences the quasineutrality. For example this field strength could be produced by two charges of $\pm 15 \mu\text{C}$ separated by 1 m. Rates of ionization and recombination can be neglected.

In conclusion one can state that the plasma is characterized by relative low density with high gradients in both, density and velocity, and generally low temperature. Furthermore collisions are not dominating, electrostatic fields of up to 5,000 V high local gradients are the main source of disturbing forces.

**4.5.3 Model**

Due to the wide range of plasma parameters none of the standard models mentioned in Section 3.2.3 can be applied directly to the current problem. Basically one can choose between a fluid or kinetic approach. The first one is not applicable in terms of a single-fluid approach as used for MHD due to the ions being simulated as kinetic particles. Pure kinetic treatment is not preferable also due to the low time base and the tremendous rise in computational time. Furthermore some of the typical electron features such as the long-tailed boltzmann distribution which are expected to be key features for the behavior of the electrons exposed to electric fields can be described in a much more suitable way in a fluid model. An argument for a kinetic approach again is that the high field gradients cause appropriate accelerations which could permit electrons to escape the cloud of the CEX particles above the solar array and form the sheath.

Two models have been developed, implemented and tested. Both combine the particle and fluid point of view.

**The kinetic density approach**

This model is based on the idea to create a kinetic flow field without the use of discrete particles. This circumvents the problem of the tremendous rise in computational times which scales with $\mathcal{O}(N^3)$ in the total number of particles for some parts of the simulation.
Kinetic aspects are necessary in order to permit electrons to escape the ion flow and follow positive potential fields emerging from the solar array, mainly the interconnectors, and account for electron backflow currents. On the relatively coarse temporal resolution collisional effects, temperatures and collective behavior can be calculated more precisely for a fluid based on the Boltzmann equation (3.11) than for discrete particles governed by fields and discrete collisions. In this way thermal movement, collisions, drifts, conservation of charge, mass, and currents are included inherently in the model.

The basic idea is to calculate flow speeds that apply to densities located at the grid points. In every time step the density at every point $p_{ijk}$ is moved virtually by its flow vector $v_{e,ijk}\Delta t_e$ and is then interpolated to the surrounding grid points by a weighting function. In order to conserve momentum and energy the weighting has to include the mass and velocity of the density fractions. In detail this method works as follows.

Starting at the basic equation of motion (3.13) using the plasma properties introduced in Section 3.2 one obtains

$$m_e n_e \frac{\partial v_e}{\partial t} + m_e n_e (v_e \cdot \nabla) v_e + e n_e E + \nabla p = \frac{en_e}{\sigma_{ei}}$$  \hspace{1cm} (4.19)

The collisional term on the right may be omitted. Using the forward discretization scheme (see Section 5.1.2) one can directly convert this equality to a discrete expression for the change in velocity $\Delta v_e$ based on the current set of data $(n_e(x,t), v_e(x,t), E(x,t), T_e(x,t))$

$$\Delta v_e = \Delta t \left[ v_e^2 n_i \sigma - (v_e \cdot \nabla) v_e - \frac{e}{m_e} E - \frac{k_B}{n_e m_e} \nabla (n_e T_e) \right]$$  \hspace{1cm} (4.20)

The fully discrete form of these three equations can be found in Section 5.3. Now that the flow speed at every point is known the move can be performed. In order to respect the continuity equation (3.12) which guarantees charge and mass conservation a method is necessary which can be represented by an operator normalized to 1. Such an operator is the trilinear interpolation already introduced for assignment of the particle density to the grid. In order to include Maxwellian velocity distributions explicitly in the model the weighting can also be done by a Maxwell-Boltzmann distribution function around the interpolation point. In either case a displacement vector $\Delta x = (v_e + \Delta v_e)\Delta t$ is calculated which gives a virtual position $x_v = x + \Delta x$. Based on this position the density originated at $x$ can be interpolated to the surrounding grid points $p_i$. Finally the weighting has to include conservation of momentum which is guaranteed by

$$\mathbf{v}_p = \frac{n_e(p)\mathbf{v}_e(p) + n_e(x) f_w(x_v, p) (\mathbf{v}_e(x) + \Delta v_e(x))}{n_e(p) + n_e(x) f_w(x_v, p)}$$

where $f_w(x, p)$ depicts the weighting function evaluated for the neighboring grid point $p$ based on the position $x$. Hence charge, momentum, and mass are inherently conserved by the algorithm.

Regarding the electron temperature the standard adiabatic model introduced for the warm plasma model and utilized in previous versions of SmartPIC (3.2.3) is used. Following [11] and [36] the adiabatic exponent $\gamma$ is set to 5/3.

The program flow takes the form depicted on the left in Figure 4.9. Preliminary results and further discussion are given in Section 4.5.4.
Figure 4.7: Kinetic density approach

(a) For each grid point \((x, y)\) the electron density \(n_e\) is moved in direction of the velocity vector \(v_e\) to a position \((x, y) + v_e \Delta t\).

(b) In the second step the density is assigned to the closest grid points by bilinear interpolation (2D example). Each point acquires a density fraction \(\Delta n_e = f_i n_e\) where \(i\) indicates the target grid point.

Heavy electron full PIC approach

In contrast to the kinetic density approach introduced in the last chapter this model uses discrete electron particles. As in the standard PIC scheme, particle properties such as density, charge, and velocity are interpolated to adjacent grid points. There the equation of motion which takes the same form as in (4.20) is solved. Resulting velocity changes are interpolated back to the particles which are subsequently moved. The great difference to the standard PIC scheme is that the particle movement is governed by fluid equations instead of the classical field acceleration scheme used for the ions. Momentum conservation is inherently given since only changes in velocities \(\Delta v_e\) are calculated according to the forces on the grid. In these calculations both, the electron mass and the interpolated velocity field on the grid are taken into account. Hence, in other words, the inertial term in (3.13) is not neglected.

The electron temperature, again, is calculated from the adiabatic energy equation. For details refer to the preceding section “Kinetic Density Model”, Section 4.5.3.

Regarding the temporal consistency discussed in Section 4.5.2 the heavy particle approach has been chosen. Since in the dense regions around the thruster exit densities of the order \(10^{17}\) are to be expected which correspond to a Debye length of \(8 \times 10^{-5}\) m the spatial resolution by far is not sufficient to resolve electron movements on a natural scale. In order to enable the electrons to follow the ion flow and maintain equilibrium the mass ratio \(m_i/m_e\) has been varied. Experimentally it was found that stability could be reached for values \(< 100\). According to the consistency condition (4.17) \(m_i/m_e = 100\) results in a time ratio of \(\Delta t_i/\Delta t_e = 10\) which is computationally feasible.

Stability analysis

The plasma potential is not calculated from the electron momentum equation by requiring \(n_i = n_e\) but obtained by directly solving the Poisson equation utilizing the FMG solver (see Section 5.3.5). This brings up the stability problems already discussed for the number densities in Section 4.5.2. The punctually high ion densities result in appropriate high local
charge differences which account for extreme potential peaks and hence, electric fields. Those fields catapult electrons to astronomical speeds at randomly seeded directions which of course leads to an indeterministic explosion of the electron cloud. That further causes electron crowds in regions not being populated by ions where large negative potentials build up causing the electrons to run back at even higher speeds into the beam. It is a circle process that builds up very rapidly.

One of the most difficult tasks in the implementation of the electron model is to find a damping mechanism for these instabilities that works reliable and does not interfere with physical correctness.

Several approaches have been tested

- smoothing the number densities of both, electrons $n_e$ and ions $n_i$
  This led to nice density distributions but killed the synchronization between the two plasma constituents completely. Electrons behaved as an independent fluid. Initially pressure forces push the electrons away which leads to a large-area potential buildup. Instabilities could not be eliminated with this method.

- smoothing the resulting potentials $\Phi$
  It turned out to be very difficult to find the right amount of smoothing. Too small values left the instability unchanged while too big ones led to the same result as for the first point.

- limiting electrical fields $\mathbf{E}$
  A simple $\Theta$ function was applied to the norm of the electric field vector, thus the force direction could be conserved while the unphysical amount was cut away. Tests showed that the optimum cutoff value is determined by simply requiring that resulting forces cannot displace an electron by more than one grid cell per ion time step. In fact the best results could be obtained with this method.

- limiting electron velocities $\mathbf{v}_e$
  This did not damp instabilities at all. It is clear that only a few electron time steps are necessary to accelerate nearly all electrons to the maximum speed. Further accelerations which would adapt the electron speed to the new distribution are prohibited. Thus no equilibrium can be found.

- varying the electron mass $m_e$
  Variation of the mass is very delicate because it not only changes the amount of inertia but also influences the necessary number of electron time steps. In fact heavier electrons behave very sluggish but the high inertia also produces massive overshooting as the electrons do not adapt very well to the ion motion.

In conclusion the best results have been obtained with limiting of the electric field to a value that does not allow the electrons to be accelerated by more than one grid cell per ion time step. For details on this see Section 4.5.4.

**Program Flow**

For completeness of the description a program flow chart including both electron fluid approaches is given in Figure 4.9 on the next page.
4.5.4 Preliminary Results

Being still in the development phase the results of the fluid model are preliminary and subject to change. Since the basic equations are the same for both models no great differences appeared in the first tests. As discussed in the previous section stable behavior of the electron fluid could only be obtained by cutting the electric field. Convergence can be seen in Figures 4.8 a–f. Initially there is a maximum difference of about $2 \times 10^{-3} \text{Cm}^{-3}$ which accounts for a differential voltage of $\approx 10^4 \text{V}$. Resulting fields theoretically range up to $10^6 \text{V/m}$ and are cut to $5 \times 10^3 \text{V/m}$. These difference are eliminated to a far extent during the first 6-8 electron time steps. Fields can effectively be reduced below 800 V/m. Despite this one can see slight overshooting in Figure 4.8 (f). In fact it is this little amount that may lead to instability.

The calculation of this short sequence which equals one ion time step on grid level 5 ($1.34 \times 10^{-7} \text{s}$) took 5 minutes on a 3 GHz Dell workstation. There is the potential to reduce this time by at least 50% by optimization.

**Figure 4.8:** Convergence in the heavy electron model. Charge density has been taken above the thruster exit every two electron cycles starting at the first cycle after ion movement.
Figure 4.9: Program flow of the fluid model. The approaches differ in the electron loop part (underlayed with dark gray). While for the kinetic density model only electron densities are inserted at the begin of a cycle in the particle approach for every ion a new electron is inserted. Forces and other fields are always calculated on the grid.
Chapter 5

Computational aspects

5.1 Numerical Methods

In order to utilize the computer to treat problems that cannot be solved exactly the specific mathematical formulation has to be discretized. In fact this opens a large field of computational mathematics that is subject to many books. The intent of this chapter is to give a very brief introduction into techniques of discretization. More detail is given to the representations of the Laplace equation and the utilized Multigrid method.

5.1.1 Introduction on Differential Equations

As many important physical processes in nature can be described by partial differential equations (PDE) the numerical treatment of these has become a central part of many scientific fields. Due to the complexity of the occurring problems the solution can often be obtained only numerically. Based on the immense rise of computational power during the last century the methods and algorithms necessary for numerical modeling have been well studied and approved. Many approaches aiming for the most efficient way to solve specific problems have been developed. Some of the most important will be discussed here.

Principally three problem classes can be distinguished by the type of PDE underlying it. These are hyperbolic, parabolic and elliptic. The prototypical example of a hyperbolic equation is the one-dimensional wave equation

\[ \frac{\partial^2 u}{\partial t^2} = \frac{1}{C^2} \frac{\partial^2 u}{\partial x^2} \]  

(5.1)

where \( u = u(x, t) \) symbols the function value at coordinates \((x, t)\) and \( C \) is a constant (in most cases the velocity of wave propagation). Hyperbolic equations typically describe so called initial value problems or Cauchy problems. Consider a spatial domain \( A \). Then \( u(x, t_0) = f_0(x) \) and \( \dot{u}(x, t = 0) = \frac{\partial f_0}{\partial t} \) must be given \( \forall x \in A \) Where \( f_0 \) is a function which gives the the initial values for \( u(x) \). The solution is the transition \( u(x)_{t=0\rightarrow T} \). For solving initial value problems numerically only the current set \( u(x, t) \ \forall x \in A \) or a few last sets have to be kept in memory.

The typical example for a PDE of parabolical type is the diffusion equation or the temperature conductance equation

\[ \frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( \frac{1}{D} \frac{\partial u}{\partial x} \right) \]  

(5.2)
with $D$ the diffusion or temperature conduction coefficient. On first sight this describes an initial value problem again. Further thinking reveals that for $t \to \infty$ the time derivative vanishes and the problem reduces to a statically one. Two types of initial value definitions can be given:

*Dirichlet* conditions

$$u(x, t = 0) = f(x) \quad \forall x \in \partial A$$

and *Von Neumann* conditions

$$\mathbf{n} \cdot \nabla u(x, t = 0) = f(x) \quad \forall x \in \partial A$$

with $\mathbf{n}$ being the unit vector perpendicular to the boundary of $A$, $\partial A$. Finally the prototype of an elliptic equation is the *Poisson* equation

$$\frac{\partial^2 u}{\partial x^2} = \rho(x) \quad \text{or in three dimensions } \Delta u = \rho(x, y, z) \quad (5.3)$$

with the source term $\rho$. The Poisson equation typically describes a static equilibrium problem or boundary value problem which has Von Neumann or Dirichlet boundary conditions.

### 5.1.2 Discretization Methods

As we know from the definition of the derivative of a function $f(x)$

$$\frac{df}{dx} = \lim_{\varepsilon \to 0} \frac{f(x + \varepsilon) - f(x)}{\varepsilon} \quad (5.4)$$

gradients are in fact limata of functions. So when transforming a problem from continuous, mathematically exact space to discretized space all one has to do is to set $\varepsilon \neq 0$. What this means in detail will be discussed now.

For convenience and to keep facts as simple as possible a rectangular grid in two dimensions $x$ and $y$, and a function $u(x, y)$ defined on all discrete points $(x, y)$ shall be assumed. The measure of the distance between two points, the *grid spacing* shall be $\Delta x$ and respectively $\Delta y$. In terms of this notation (5.4) can be written as

$$\frac{\partial u}{\partial x} = \lim_{\Delta x \to 0} \frac{u(x + \Delta x, y) - u(x, y)}{\Delta x} \quad (5.5)$$

In practice the limes has to be omitted when working with discrete grid spacings. In that case the error can be estimated as follows.

If one Taylor-expands $u(x_0 + \Delta x, y_0)$ around $(x_0, y_0)$ the result is

$$u(x_0 + \Delta x, y_0) = u(x_0, y_0) + \frac{\partial u}{\partial x}|_{x_0} \Delta x + \frac{\partial^2 u}{\partial x^2}|_{x_0} \left(\frac{(\Delta x)^2}{2!}\right) + \ldots + \frac{\partial^n u}{\partial x^n}|_{x_0} \left(\frac{(\Delta x)^n}{n!}\right) \quad (5.6)$$

When breaking after the first derivative term one obtains directly

$$\frac{\partial u}{\partial x}|_{x_0,y_0} = \frac{u(x_0 + \Delta x, y_0) - u(x_0, y_0)}{\Delta x} + \text{T.E.} \quad (5.7)$$

where the truncation error (T.E.) is $O(\Delta x)$. This is legitime and confirmed by the mean value theorem which ensures that the approximation (5.7) is exact for at least one $x' \epsilon [x, x + \Delta x]$. The only thing one has to take care of is the convergence of the T.E. Equation (5.7) is called the *forward finite difference representation* of the derivative (5.4). *Forward* because
of the positive orientation of $\Delta x$ relative to $x_0$. All this can be proven explicitly. For
details to that please refer to [37].
Spatial coordinates in the finite difference representation are given in units of the grid
spacing by the notation
\begin{equation}
  u(i\Delta x, j\Delta y) \equiv u_{ij}
\end{equation}
According to (5.7) it can also be defined the backward finite difference representation
\begin{equation}
  \frac{\partial u}{\partial x}|_{ij} = \frac{u_{ij} - u_{i-1,j}}{\Delta x} + O(\Delta x)
\end{equation}
and finally the central difference
\begin{equation}
  \frac{\partial u}{\partial x}|_{ij} = \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x} + O(\Delta x)
\end{equation}
If proceeding the same way for the 2nd derivative one obtains
\begin{equation}
  \frac{\partial^2 u}{\partial x^2}|_{ij} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{ij}}{(\Delta x)^2} + O[(\Delta x)^2]
\end{equation}
This is almost the basis for the finite difference representation of the Poisson or Laplace
equation (5.3). The finite difference method is only one among a number of discretization schemes. Any
further detail is beyond the scope of this work. A more comprehensive and detailed
treatment of this thematic can be found in [38].

5.1.3 Relaxation methods
Relaxation methods are iterative schemes used to propagate disturbances or function
extrema throughout a computational domain following given physical laws. Thus they
smooth or relax the function of interest. The simplest and most intuitive method is Gauss-Seidel or Jakobi. For explanation one
should start from an explicit 2-dimensional example
\begin{equation}
  u_{ij}^{t+1} = \frac{u_{i-1,j}^{t+1} + u_{i+1,j}^{t+1} + u_{ij}^{t+1} + u_{ij-1}^{t}}{4}
\end{equation}
With $t$ being the discrete time index. Obviously this is a simple mean value calculation.
One thing that is special here is the usage of $u_{ij}^{t+1}$ expressions on the right hand side. This
follows from the iteration order which goes $i : 1 \rightarrow i_{\text{max}}, j : 1 \rightarrow j_{\text{max}}$. Points with smaller
indices than the currently processed point have already been assigned an updated value.
If this continuous updating of values takes not place the method is called Jakobi which
practically needs twice as many iterations as Gauss-Seidel. More general the Gauss-Seidel
scheme can be written in one dimension as
\begin{equation}
  u_i^{t+1} = \frac{1}{L_{ii}} \sum_{j=1, j \neq i}^{N} L_{ij} u_j - f_i
\end{equation}
where $N$ is the number of grid points and $L_{ij}$ is a linear differential operator acting between
points $i$ and $j$.
The great drawback of this method is the very slow convergence rate due to propagation
limited by the grid spacing $\Delta x$ which is embedded in the differential operator. At this point some more advanced methods as the successive overrelaxation (SOR) attach. Instead of calculating the linear mean value SOR introduces an overrelaxation factor $\Omega$ which multiplies the change of the value. $\Omega$ has to be chosen very carefully in order not to produce uncontrolled overshooting. Additionally the factor can be adapted from one iteration to another leading to optimized convergence rates many times higher than simple Gauss-Seidel iteration. Just to give a hint of how SOR works I would like to give a short sketch of it

$$ u^{l+1}_{i,SOR} = \Omega u^{l+1}_{i,GS} + (1 - \Omega)u^l_i $$

(5.13)

where $u_{i,SOR}$ is the solution for the SOR iteration, and $u_{i,GS}$ is the Gauss-Seidel result given by (5.12). It can be shown that the method only converges if $\Omega \in [0, 2]$. For $\Omega = 1$ SOR reduces to simple Gauss-Seidel. More on this method can be found in [39] and [38].

5.1.4 Multigrid method

Multigrid methods are the fastest to solve arbitrary linear or nonlinear PDEs universally. Of course for very specific problems direct methods as matrix inversion or partially analytic schemes can be found but barely any method is able to catch up in speed with multigrid methods for such a broad spectrum of problems.

The basic idea is to speed up convergence of classical iteration schemes mentioned in Section 5.1.3 by computing the problem on several levels of different grid spacings. Thus the low frequency disturbances on fine grid levels which propagate very slowly are transformed to high frequency components on the coarse grid levels where they spread throughout the computational domain very fast. Convergence can be achieved in $O(N)$ operations (where $N$ is the number of points on the finest grid). As most textbooks propose, for explanation one should start with the basics shown on a two-grid variant.

Mathematical definitions

The multigrid method requires deeper knowledge of approximation errors and their exact definitions. For simplicity all operators are introduced in their 2-dimensional form. To keep this section more general a universal linear operator $L$ is introduced that acts on discrete gridpoints numbered by $i \in [1, N] \subset \mathbb{N}$. The most uniform representation of this operator is

$$ Lu_{ij} = f_{ij} $$

(5.14)

with $u$ the sought potential and $f$ the source- or disturbance term. Due to the fact that the approximate solution $\tilde{u}^t_{ij}$ only converges against the exact solution $u_{ij}$ in the limes $t \rightarrow \infty$ one can define the error $\Delta u^t_{ij}$ as follows

$$ u_{ij} = \tilde{u}^t_{ij} + \Delta u^t_{ij} $$

(5.15)

Since $L$ is a linear operator it follows further

$$ Lu_{ij} = L\tilde{u}^t_{ij} + L\Delta u^t_{ij} $$

(5.16)

Here one can define the residual as

$$ R_{ij} = L\tilde{u}^t_{ij} $$

(5.17)
which must fulfill the relation $\tilde{u}_{ij} \rightarrow u_{ij} \Rightarrow R_{ij} \rightarrow 0$. The residual is the result of (5.14) if the left hand side is evaluated with the approximate solution $\tilde{u}_{ij}$. Thus (5.16) becomes

$$Lu_{ij} = L\Delta u_{ij}^t + R_{ij}^t$$

(5.18)

For simplicity at this point $f_{ij}$ is assumed to be 0. Otherwise it would be written as an additional term on the right. Assuming this one can state that

$$-R_{ij}^t = L\Delta u_{ij}^t$$

(5.19)

from which one can easily calculate the error $\Delta u_{ij}^t$.

In order to calculate residual and error on all grid levels transformation operators are needed. Levels of different grid spacing are numerated from 0 at the coarsest level to $M$ for the finest level. For transformation from a fine grid of level $m$ to the next coarser grid $m - 1$ the restriction operator $R_{m-1}^m$ is used. The simplest coarsification is direct insertion where the values $\Delta u(m)$ are just copied to the corresponding points on the coarse grid $\Delta u(m - 1)$. Increasing the number of points taken to interpolate the coarse grid value half weighting and full weighting are very useful. It is clear that accuracy is enhanced the more fine grid points are taken into account when interpolating.

$$R_d = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad R_{hw} = \begin{pmatrix} 0 & \frac{1}{8} & 0 \\ \frac{1}{8} & \frac{7}{8} & \frac{1}{8} \\ 0 & \frac{1}{8} & 0 \end{pmatrix} \quad R_{fw} = \begin{pmatrix} \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \end{pmatrix}$$

(5.20)

Going the other way from coarse to fine grid levels one needs an Interpolation operator or Prolongation operator $I_{m+1}^m$. For this operation the same considerations as for restriction are valid: The more points are taken into account for interpolation the higher the resulting accuracy is. In addition an operator of higher dimension leads to a higher convergence rate. The most popular interpolation method is multilinear interpolation which equals for two dimensions the bilinear interpolation

$$I_{bi} = \begin{pmatrix} \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{4} & \frac{1}{2} & \frac{1}{4} \end{pmatrix}$$

(5.21)

Basically there are two versions of the multigrid method: The iterative multigrid method and the full multigrid method FMG.

**Iterative multigrid method**

The iterative method uses the different levels to calculate and summarize the errors occurring on the finest grid. The basic steps of the method are

- (5.14) is solved on the finest level by utilizing a classical relaxation method as Gauss-Seidel $n > 1$ iterations, starting with $u_{ij} = 0 \forall ij$ as initial guess. Thus one obtains a first approximate solution $\tilde{u}_{ij}$.

**Remark:** It is very important not to use SOR here because the overrelaxation cuts high frequency components in the spectrum of the function which has to be propagated. This is common to all versions of the multigrid scheme.
The residual (5.17) is calculated for every point and stored as $R_{ij}^M$ where the $M$ denotes the number of the finest level. Time indices will not be used here.

Restriction of the residual to the next coarser level by

$$R_{ij}^{M-1} = R_{M}^{M-1}R_{ij}^M. \quad (5.22)$$

This coarsification can now be used to solve (5.17) for the error $\Delta u_{ij}^{M-1}$, by utilizing Gauss-Seidel again for a few iteration sweeps. $\Delta u_{ij}$ represents now the correction to the finest grid solution $u_{ij}^M$. The residual has to be updated previously to restricting it to the next coarser level in order to propagate the high frequency components of the fine level.

$$R_{ij}^{M-1} = R_{M}^{M-1}R_{ij}^M + L\Delta u_{ij}^{M-1} \quad (5.23)$$

$R_{ij}^{M-1}$ has to be restricted to the next coarser level $M-2$.

On the coarsest grid Equation (5.17) is iterated to convergence giving the solution for the error $\Delta u_{ij}^0$. This will not take much time because the coarsest level should yield just as much points as necessary to include all boundary conditions.

Now the error values represent the necessary corrections to the solution $\tilde{u}_{ij}$ on the coarsest grid level 0. These corrections have to be interpolated to the next finer level utilizing

$$\Delta u_{ij}^1 = I_{0}^1\Delta u_{ij}^0 \quad (5.24)$$

The interpolated corrections are to be added to those obtained in the restriction phase earlier

$$\Delta u_{ij}^{1,new} = I_{0}^1\Delta u_{ij}^0 + \Delta u_{ij}^1 \quad (5.25)$$

This correction now represents the corrections necessary on grid level 0 and level 1. The next step is interpolation of $\Delta u_{ij}^{1,new}$ to level 2.

The last two points are processed iteratively until the finest grid level $M$ is reached.

After obtaining $\Delta u_{ij}^{M,new}$ the accumulated corrections are added to the approximated solution $\tilde{u}_{ij}^M$.

Finally a small number $n$ sweeps of Gauss-Seidel are processed on the solution (5.14).

At this point a complete multigrid cycle up and down all levels of the hierarchy is completed. If the solution does not fulfill the convergence criteria a new cycle is started beginning with the first point but taking the results of the first run $\tilde{u}_{ij}^M$ as initial guess for Gauss-Seidel.

Practically only a few multigrid cycles are necessary to obtain a well converged solution.
Full multigrid method

Iterative multigrid is the simplest scheme to use the advantages of multigrids. In fact it is not the fastest one. The scheme presented in this section takes maximum advantages of the multigrid scheme, thus resulting in very short run times. Basically the two methods presented differ in three points.

- initial guesses
- accumulation of corrections
- the way boundary conditions and sources enter the calculation

First FMG does not start on the finest grid level but on the coarsest one. There the exact solution is sought and found very quickly because of the very limited number of grid points. This brings the advantage to start from values much closer at the converged solution than the initial guess 0 for the iterative method.

Secondly point the corrections are not only accumulated when stepping from coarse to fine levels but also smoothed by a relaxation method like Gauss-Seidel. Finally instead of running down and up the entire depth of the level hierarchy \([0..M]\) for every cycle an increasing depth \(n_{\text{max}}(k) = k + 1\) with \(k\) stepping from 0 to \(M\) is used. One can picture this scheme easily as in Figure 5.1. The source term and boundary conditions enter the calculation at the coarsest level when solving exactly for the first time and at the finest level of each “V”. There the residual is newly calculated from the source and boundary on the current grid level. This requires knowledge of the source as well as the boundary on every level. In practice it is not sufficient to just restrict \(f_{ij}\) to coarser levels. It has to be redefined on every level to meet the physical conditions.

Explicitly the FMG scheme processes the following steps

- Starting at the coarsest level 0 (5.14) is iterated to convergence.
- This rough solution is interpolated to level 1 by

\[
\tilde{u}^1_{ij} = I^1_0 \tilde{u}^0_{ij}
\]  

(5.26)

and relaxed by a few sweeps of Gauss-Seidel. The first V differs at this point from all further ones. Here the solution \(\tilde{u}^0_{ij}\) is solved at and interpolated from the coarsest level. Later the error will treated in the same manner.
• On level 1 the residual $R_{ij}^1$ (5.17) can be calculated as was done for the iterative method taking $\tilde{u}_{ij}^0$ as initial guesses. The error is obtained by Equation (5.19).

• From this point on the FMG does not differ much from the iterative scheme. The error is restricted, relaxed and added to the residual on each level. Additionally a few sweeps of Gauss-Seidel are processed on (5.19). This procedure is called Pre-Smoothing because it relaxes the residual previously to interpolating it to the next coarser level.

• Restricting, accumulating and relaxing is continued until the coarsest level is reached. There the error is solved exactly as was done for the initial solution in the first step.

• Entering the prolongation phase the error is interpolated to the next finer level and added to the error obtained earlier in the restriction phase (5.25).

• This new error is again relaxed by applying Gauss-Seidel on (5.19) which is now called Post-Smoothing.

• At this point it is optional if the solution shall finally be known exactly on each level or just on the finest one. If $u_{ij}^k$ is required for every $k \in [0..M]$ the correction $\Delta u_{ij}^n$ is added to $\tilde{u}_{ij}^n$ obtained by interpolation from the coarse grid solution at the beginning of the current $V$-cycle. This can be done on each level after each interpolation step, thus resulting in a complete solution for every level $n$. If this is not necessary one can save some little time in just proceeding to the next finer level without recalculating the solution.

• This procedure of interpolation, addition and relaxation is iterated until the currently finest level $n_{\text{max}}(k)$ is reached where the accumulated error now has to be added to the solution.

• In order to make the step from the $n$-staged $V$ to deeper ones the solution $\tilde{u}_{ij}^{n_{\text{max}}(k)}$ has to be interpolated to level $k + 1$. There a new $V$-cycle starts by calculating a new residual $R_{ij}^{n_{\text{max}}(k) + 1}$ and the appropriate error $\Delta u_{ij}^{n_{\text{max}}(k) + 1}$.

• With each $V$-cycle the solution is known one level deeper in the hierarchy. Finally the result is $u_{ij}^M$ (and optionally all other solutions $u_{ij}^k$).

Convergence can be used as criteria to decide if a second run is necessary but practice has shown that it is sufficient to adapt the number of sweeps for Pre- and Post-Smoothing and coarse grid exact solution. Additionally on each level two or more $V$-cycles can be processed. In fact numbers for relaxation sweeps are well below 10 and in most cases only one $V$ per level is needed to obtain good solutions. A detailed procedure how to determine those numbers practically can be found in [39]. More theoretical guidance is given by [40].

5.1.5 Particle in Cell

The Particle in Cell (PIC) scheme is a method to simulate huge amounts of particles governed by macroscopic forces in reasonable time. The trick has already been discussed in Section 4. Once again, great numbers of physical particles are represented by a computational super particle. The ratio of real particles per virtual particles (PPP) used in SmartPIC is $10^8 - 10^{10}$ depending on the type. CEX ions are subject of investigation and need to be resolved on a fine scale ($PPF_{\text{CEX}} = 2 \times 10^8$). Neutrals only influence
the plasma behavior by their density which scales the probability for collisions, hence they are treated with a high PPP ratio \(PPP_n = 1 \times 10^{10}\). Beam ions are treated at \(PPP_i = 5 \times 10^9\).

The essential part of the PIC scheme is the changing point of view between grid and particle. Figure 5.2 clarifies the process. Particles are the carrier of energy, charge, and mass. They move on physically correct paths creating a flow field. The resulting densities, velocities, and currents are interpolated to 8 points defining the grid cell a particle is situated in. This weighting is done by trilinear interpolation depending on the absolute distance to each point. Based on the interpolated particle properties the electric potential, electric field, gas pressure, momentum, and temperature can be calculated at every grid point. These fields are interpolated back to the particle positions and converted into a change in velocity.

5.1.6 Leap Frog

This scheme is based on the Verlet algorithm. It brings major advances in energy conservation which is generally a problem in PIC simulations. The principle is that forces are calculated temporarily shifted to particle movements. This has the effect of temporal smoothing.

In detail one can start with the Taylor expansion of the position \(x(t + \Delta t)\) and \(x(t - \Delta t)\); subtraction results in

\[
x(t + \Delta t) = 2x(t) - x(t - \Delta t) + \frac{\partial^2 x}{\partial t^2} \bigg|_t (\Delta t)^2
\]

This represents an equation of motion including particle positions at times \(t\) and \(t - \Delta t\). It has an error of \(O[(\Delta t)^4]\) which is quite good.

For the velocity \(v\) the standard centered discrete temporal derivation \(\Delta x(t)/\Delta t\) of the form (5.10) is backed with an error \(O[(\Delta t)^2]\) which can be reduced to 1/4 by using \(\Delta t/2\) steps.

\[
v(t + \frac{\Delta t}{2}) = v(t - \frac{\Delta t}{2}) + \frac{\partial v}{\partial t} \bigg|_t \Delta t
\]

If one rewrites the centered discrete first derivation of \(x(t)\) to

\[
x(t + \Delta t) = x(t - \Delta t) + v(t)2\Delta t
\]

and replaces \(\Delta t\) by \(\frac{\Delta t}{2}\), and sets the reference \(t\) to \(t + \frac{\Delta t}{2}\) one obtains finally

\[
x(t + \Delta t) = x(t) + v(t + \frac{\Delta t}{2})\Delta t
\]  \hspace{1cm} (5.27)
which is the equation of motion for the leap frog algorithm.

5.2 Grid generation

The type and metric of the computational grid is a very basic and important factor in simulations. Depending on the type of equations that have to be solved the grid directly influences the form of operators and the algorithms that work on the grid. Principally grids can be classified by their structure.

5.2.1 Grid Types

Structured Grids

Structured grids use special transformations to simplify the domain of interest into a regular computational grid on which the solution is calculated. After finding a solution data have to be transformed back onto the physical grid. The transformation affects the form of operators and algorithms. Hence a reasonable computational effort has to be spent on that. One major drawback of structured grids is that most of the adaption work has to be done analytically and mesh generators are bound to the geometry of the current problem. Every change in boundaries goes along with design changes in the code. On the other hand structured grids provide high quality in accuracy of the solution. Since they are adapted optimally to the geometry and inherently support the expected form of the solution very low noise and extraordinary convergence can be attained. Structured grids have been used by [8] et al.

Theoretical guidance can be found in most textbooks on simulation techniques and meshing (for example [38]).

Unstructured Grids

This type of grids does not distribute its points according to any ordered scheme but tries to keep the volume of each cell constant. Several methods have been developed to achieve this.

The great advantage of unstructured grids is that they can be generated automatically.
and adapt to a far extent to arbitrary boundary geometries. In contrast to the structured schemes connectivity information (face-face, or cell-cell) has to be stored for every point in the grid. Since computer memory is cheap today, this is no problem. Other side-effects weight much more in this case. First due to the grid being inherently not adapted to the expected form of the solution much more cells are produced than are necessary for a structured grid (approximately factor 5). Secondly computational noise is quite high and equation solver algorithms cannot be very efficient due to ever changing grid spacings and non-orthogonality. Principally unstructured grids are applied in automatic grid generation systems and in simulations where exactness of field solutions is not the primary element, for example Monte Carlo collision models.

Alternative Approaches

For some special configurations alternate methods are applied. One approach is mixing of structured and unstructured grids where the analytically adapted grid is implemented for boundary regions and the unstructured grid to fill the rest of the domain. Such combinations have been successfully utilized in the past, for example airfoil flow simulations. Another approach is called domain subdivision. Basically rectangular grids are used which are iteratively divided in boundary regions until the adaption reaches the desired level. This approach is rather simple but allows high accuracy at boundaries despite not orienting grid faces to surfaces. This concept will be extended in Section 5.2.2.

5.2.2 Semi-adaptive multigrid

The requirement for a fast and simple algorithm enforces to use a rectangular type grid. On such the standard five-point form of the Poisson equation (see Section 5.3) can be used. This, in accordance to the problem, represents the simplest possible form for that type of equation. In addition a rectangular grid eases the generation of multi-layers or levels of different grid spacings which are an essential requirement for application of the multigrid solver.

Domain Creation: simple version

These baselines are easy to implement. One has to start at some initial point and fill the computational domain with points of equal orthogonal spacing. Let the subdivision factor be 2, then the next level is introduced by inserting 7 new points for each existing one. This

![Figure 5.4: Creation of a fine grid cell with the base point P_{ijk} by grid division](image)

Figure 5.4: Creation of a fine grid cell with the base point $P_{ijk}$ by grid division
method works fine and can be conducted throughout the grid - except for the $+X$, $+Y$, and $-Z$ borders where no complete cubes can be attached to the base point. In addition to insertion of points the navigation structure has to be initialized for each point. This will be explained next.

**Navigation**

One of the major features of the programming language C/C++ are *pointers*. These are references to structured memory blocks called *objects*. In SmartPIC grid points are defined as such objects offering direct access to all grid based physical properties.

Navigation through the grid is an essential thing. In older versions of the simulation grid points have been arranged in a one-dimensional array $P(n)$, requiring recalculation of the coordinates $(i, j, k)$ into an array number $n$.

$$n = iN_x + jN_y + zN_z$$

where $N_a$ gives the total number of gridpoints in direction $a$. Hence access to the next neighbor grid point takes 3 multiplications, 2 additions and one access operation. This type of access is needed for all iterative schemes in the multigrid solver and other parts in the program. For the current program version a more efficient navigation method has been implemented. Each point $P$ possesses 6 navigation pointers. These are initialized while generating the grid. The grid pointers refer to the next neighbors available on the current level. At domain borders, where no next neighbors exist, so called *loopback pointers* are introduced. These are very important because they inherently define the Von Neumann condition $\nabla_n f = 0$ with $\nabla_n$ being the derivation of an arbitrary function $f$ in direction of the boundary surface normal $n$.

Compared to the array-based method mentioned earlier the pointer navigation needs only one single access operation in order to get a neighbored grid point. This means an enormous advantage in speed.

In addition to the 6 navigation pointers a so called *iteration pointer* is introduced. Its purpose is to speed up iteration for relaxation algorithms. As discussed in Section 5.1.3 the iteration order can take advantage of the fact that some values $u_{ijk}^{t+1}$ of the smoothed function are already known. Several schemes can be applied. Values can be updated row by row, line by line, or by so called “red-black” (also referred to as “checkerboard”) ordering where in the first step all red points are updated and in the second all black ones. These schemes had a great influence on computing time in so called “vector” machines. Those were designed to execute several operations of the same type simultaneously. The
crucial thing about this was that all input parameters had to be known previously to execution. If one variable depends on the result of a recent calculation the parallel execution did not work. That’s the reason why schemes have been implemented not using a newly calculated variable in the next step.

In current computer architectures this is not a big problem any more due to the so-called “multi stage pipelines” where a result can be inserted into the line of executions within 2 or 3 steps depending on the architecture. Since one relaxation step in the schemes presented here consists of definitely more than 3 operations the influence of iteration schemes on speed is lost.

In SmartPIC the iteration order has been optimized for shortest iteration in nested loops.Domains including the solar array are y-ordered (in Figure 5.6), all others are z-ordered. This scheme guarantees short iteration times because the program (at run time) does not need to care about which point to get next or to check boundaries. Moreover the crosswise iteration assures smooth propagation, and hence reduces errors.

**Grid Domains** The generation scheme introduced in Section 5.2.2 works well for a uniform grid, filling the entire computational domain. Since in order to reach a resolution fine enough to resolve interconnector structures a grid size of $\Delta x \approx 8.59\, \text{mm}$ has been chosen. A rough estimate for the $2\, \text{m} \times 7.5\, \text{m} \times 2\, \text{m}$ domain gives $4.73 \times 10^7$ grid points solely for the finest level. At 360 Bytes per grid point the grid alone would take 15.9GB of memory which is not feasible with a standard workstation. Additionally most of these points are situated in regions of the domain where such a high resolution is not necessary.

The solution is to build nested domains. The domains of the finest level have to cover the smallest volume. In each coarser level the size of the domain grows until the whole computational domain is included on the coarsest level.

In order to provide a good fit to the spacecraft the initial grid size is chosen to be $1/4$ th of the spacecraft main body’s $x$-dimension. This results in $\Delta x_0 = 275\, \text{mm}$ according
to the input parameters declared in Section 2.2, Table 2.1. Starting on the coarsest level number 0 the level grid sizes $\Delta x_{1.5}$ are obtained by iteratively dividing by 2.

**Remark:** The number of 6 levels has been assumed in an early phase of implementation and has proven to give good results. It could be changed to attain even finer resolution if necessary.

A grid domain is defined by its entry grid point and the number of grid cells in all three directions. Thus it is possible not to fill the entire computational domain on each level but to shrink domain sizes on each level around points of interest. In order to minimize errors the grid boundaries of a domain of level $n$ must have a distance of at least $2\Delta x_{n-1}$ to the next boundary on level $n-1$.

<table>
<thead>
<tr>
<th>Level</th>
<th>$\Delta x$ [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>275.0</td>
</tr>
<tr>
<td>1</td>
<td>137.5</td>
</tr>
<tr>
<td>2</td>
<td>68.75</td>
</tr>
<tr>
<td>3</td>
<td>34.375</td>
</tr>
<tr>
<td>4</td>
<td>17.1875</td>
</tr>
<tr>
<td>5</td>
<td>8.59375</td>
</tr>
</tbody>
</table>

**Table 5.1:** Grid Sizes

Solar Array Adaption For the solar array domains of maximal level (minimal grid size) adapt to the rotation. The scheme is optimized for each octant. In Figure 5.7(a) the domain ordering for horizontal positions ($0^\circ < \alpha \leq 45^\circ$, $135^\circ < \alpha \leq 180^\circ$) with vertical domain attachments is depicted. (b) shows the scheme for vertical solar array positions ($45^\circ < \alpha \leq 135^\circ$). Based on the parameters Height, Tolerance, $\alpha$, and the grid level the adaption has to be performed. The number of domains for completely covering the solar array is varied accordingly. Domains are aligned stepwise in order to respect Height and Tolerance. Additionally the algorithm has to assure that higher level domains fit into existing coarser domains with some overlap.

Points of interest Two areas have to be treated at maximum resolution. This is the thruster exit and at least the central region of the plume, and the surface of the solar array. Both are supplied the highest spatial resolution by domains of level 5. However in order to reduce memory requirements to a minimum the sizes of these domains have been restricted to a distance of 4 cells (3.44 cm) from the dielectric surface of the solar array, and 64 cells (55 cm) in positive z direction from the thruster exit. Exemplary figures for the domain distribution are given in the Appendix, Figures B.1 – B.3, and B.4 – B.9.

Computational domain The computational domain is constructed to include one half of SMART–1 cut by the plane defined by the $x$, and $z$-axis. Spacings between the satellite and domain boundaries are chosen in a way to minimize errors due to mirroring (see Section 4.3.1), and on the other hand require a minimum number of grid points. In total the dimensions are $(DDS_x \times DDS_y \times DDS_z) = (2.2 \text{ m} \times 7.5 \text{ m} \times 2.2 \text{ m})$ including approximately 1,300,000 grid points. Basic sizes can be seen in Figure 5.8.
5.3 Explicit Implementation of the Numerical Methods

The intention of this section is to document the explicit realization of the methods introduced above. First the finite difference representation for the Poisson equation and three-dimensional operators for interpolation and restriction will be deduced. Finally a modified version of the FMG scheme for calculation of the electric potential distribution will be presented.

5.3.1 Discretization of the Poisson Equation in Detail

The way discretization is done is governed by the kind of equation and the type of computational grid on which the solution shall be obtained. The Poisson equation (5.3) is an
The Poisson equation can be written in components as an elliptical partial differential equation of second order. So for a discrete representation one needs a formulation for the second spatial derivatives. The utilized grid is rectangular in three dimensions with equal grid spacings $\Delta x = \Delta y = \Delta z$. As discussed in chapter 5.1.2 a finite difference representation under such conditions can be obtained by a Taylor series expansion.

The Poisson equation can be written in components as

\[
\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = -\frac{\rho}{\epsilon_0}
\]  

(5.28)

Since for Gauss-Seidel on a rectangular grid for each point $p_{i,j,k}$ six next neighbors can be found, each at a distance of one step $\Delta x$ in positive and negative direction on each coordinate line. Thus a centered difference representation for the derivatives can be utilized. I will give the explicit calculation for the coordinate $x$ respectively index $i$.

For the centered representation of $\frac{\partial^2 u}{\partial x^2}(i,j,k)$ expansions for $u_{i-1,j,k}(u_{i,j,k}, \Delta x)$ and $u_{i+1,j,k}(u_{i,j,k}, \Delta x)$ are needed.

\[
u_{i-1,j,k} = u_{i,j,k} - \frac{\partial u_{i,j,k}}{\partial x} \Delta x + \frac{1}{2!} \frac{\partial^2 u_{i,j,k}}{\partial x^2} (\Delta x)^2 - \frac{1}{3!} \frac{\partial^3 u_{i,j,k}}{\partial x^3} (\Delta x)^3 + \ldots
\]

(5.29)

\[
u_{i+1,j,k} = u_{i,j,k} + \frac{\partial u_{i,j,k}}{\partial x} \Delta x + \frac{1}{2!} \frac{\partial^2 u_{i,j,k}}{\partial x^2} (\Delta x)^2 + \frac{1}{3!} \frac{\partial^3 u_{i,j,k}}{\partial x^3} (\Delta x)^3 + \ldots
\]

(5.30)

Adding these two equations one obtains

\[
u_{i+1,j,k} + \nu_{i-1,j,k} = 2u_{i,j,k} + \frac{\partial^2 u_{i,j,k}}{\partial x^2}(\Delta x)^2\left|\frac{1}{12} \frac{\partial^4 u_{i,j,k}}{\partial x^4}(\Delta x)^4 + \ldots\right.
\]

(5.31)

The term of fourth order is omitted and represents the maximum of the truncation error. Simple calculation gives further

\[
\frac{\partial^2 u_{i,j,k}}{\partial x^2} \approx \frac{u_{i-1,j,k} - 2u_{i,j,k} + u_{i+1,j,k}}{(\Delta x)^2} + \frac{1}{12} \frac{\partial^4 u_{i,j,k}}{\partial x^4}(\Delta x)^2
\]

(5.32)

It is important to notice that the truncation error now is of the order $O\left[(\Delta x)^2\right]$. Complete in three dimension the equation takes the form

\[
\Delta u_{i,j,k} \approx \frac{u_{i-1,j,k} + u_{i+1,j,k} + u_{i,j-1,k} + u_{i,j+1,k} + u_{i,j,k-1} + u_{i,j,k+1} - 6u_{i,j,k}}{(\Delta x)^2}
\]

(5.33)

### 5.3.2 Discretization of the Electron Momentum Equation

The principal method for calculation of the change in the electron velocity $\Delta \mathbf{v}$ is the same for both proposed electron fluid models. See Section 4.5.3 for details on the model and explanation of the symbols. Since SmartPIC utilizes a cartesian coordinate system the components $\Delta v_x$, $\Delta v_y$, $\Delta v_z$ are calculated separately.

\[
\Delta v_{x,i,j,k} = \Delta t_e \left( -v_{x,i,j,k} \frac{v_{x,i+1,j,k} - v_{x,i-1,j,k}}{2 \Delta x} - v_{y,i,j,k} \frac{v_{x,i,j+1,k} - v_{x,i,j+1,k}}{2 \Delta y} - v_{z,i,j,k} \frac{v_{x,i,j,k+1} - v_{x,i,j,k-1}}{2 \Delta z} - \frac{k_B}{m_e} \frac{T_{e,i,j,k} n_{e,i,j,k} - n_{e,i-1,j,k}}{2 \Delta x} + \frac{T_{e,i,j+1,k} - T_{e,i-1,j,k}}{2 \Delta x} + \frac{e}{m_e} F_{x,i,j,k} + v_{e,i,j,k}^2 n_{e,i,j,k} \sigma_{el} \right)
\]

(5.34)
\[\Delta v_{y,i,j,k} = \Delta t_e \left( -v_{x,i,j,k} \frac{v_{y,i+1,j,k} - v_{y,i-1,j,k}}{2\Delta x} - v_{y,i,j,k} \frac{v_{y,i,j+1,k} - v_{y,i,j+1,k}}{2\Delta y} + v_{z,i,j,k} \frac{v_{y,i,j,k+1} - v_{y,i,j,k-1}}{2\Delta z} - k_B \frac{T_{e,i,j,k} n_{e,i,j,k} - n_{e,i,j-1,k}}{2\Delta y} + \frac{e}{m_e} E_{y,i,j,k} + v^2_{e,i,j,k} n_{i,j,k} \sigma_{ei} \right) \] (5.35)

\[\Delta v_{z,i,j,k} = \Delta t_e \left( -v_{x,i,j,k} \frac{v_{z,i+1,j,k} - v_{z,i-1,j,k}}{2\Delta x} - v_{y,i,j,k} \frac{v_{z,i,j+1,k} - v_{z,i,j+1,k}}{2\Delta y} + v_{z,i,j,k} \frac{v_{z,i,j,k+1} - v_{z,i,j,k-1}}{2\Delta z} - k_B \frac{T_{e,i,j,k} n_{e,i,j,k+1} - n_{e,i,j,k-1}}{2\Delta z} + \frac{e}{m_e} E_{z,i,j,k} + v^2_{e,i,j,k} n_{i,j,k} \sigma_{ei} \right) \] (5.36)

5.3.3 Restriction and Interpolation Operators

Both restriction and interpolation are to be computed in three dimensions. Practice has shown that the utilized operators have a great influence on the quality of the results. The restriction operator mainly effects the propagation of fine grid errors on coarser grids. Optimal results have been achieved for \(R_{\text{M}^{-1}}\) being the exact adjoint of \(T_{\text{M}^{-1}}\). Thus the method of full weighting had to be implemented which uses 26 adjacent points instead of only 6 for half weighting \(R_{\text{hw}}\). See Equation (5.20) for details.

Explicitly the restriction operator has the form

\[R_{\text{hw},1jk} = \begin{pmatrix} \frac{1}{64} & \frac{1}{32} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{32} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \end{pmatrix} \quad R_{\text{hw},2jk} = \begin{pmatrix} \frac{1}{32} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{16}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \end{pmatrix} \quad R_{\text{hw},3jk} = \begin{pmatrix} \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{16}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \\ \frac{1}{16} & \frac{1}{16} & \frac{1}{16} & \frac{1}{16} \end{pmatrix} \] (5.37)

Trilinear interpolation was chosen as operator for Prolongation.

\[I_{\text{tri},1jk} = \begin{pmatrix} \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \end{pmatrix} \quad I_{\text{tri},2jk} = \begin{pmatrix} \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \end{pmatrix} \quad I_{\text{tri},3jk} = \begin{pmatrix} \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{8} & \frac{1}{8} & \frac{1}{8} \end{pmatrix} \] (5.38)

5.3.4 The Poisson Source Term

The multigrid solver requires a self-consistent source term on the right side of the Poisson equation. In order to achieve this, one has to critically rethink, again, the principle of densities and the Poisson equation.

The concept of densities has been reviewed in Section 4.5.2. The conclusion is that in order to use densities one has to assure that the number \(N\) of instances involved in the density calculation fulfills \(N \gg 1\). On the other hand the Coulomb law is only exact for single infinite small charges, point charges. So for densities the principle of discrete superposition had to be applied. In the simulation the problem can be described as follows.

Let \(P\) be a single particle of charge \(q\) situated in a grid cell of arbitrary level \(n > 0\) with a grid size \(\Delta x_n\). For simplicity let the problem be 1-dimensional. Let the position of \(P\) be exactly in the middle of the cell. Then the charge density which has to be set to the
surrounding grid points is $\frac{2}{3}(\Delta x_n)^{-1}\text{m}^{-1}$. If one compares the result obtained with the charge density to the distribution for a point charge there is a definite error. The error comes from the fact that on the coarse level solution one has to assume a uniform charge distribution over a volume $\Delta x_n$ which is not the case. Thus there is a spreading of the potential solution. This is the main source of error in the calculation of potentials (see Section 5.4).

![Figure 5.9](image)

**Figure 5.9:** Spreading of the coulomb potential due to treatment on different levels. The coarse grid solutions on level $n$ are based on a uniform charge distribution over one unit cell of length $\Delta x_n$. When interpolating to fine grids the potential is too high, compared to the fine grid solution.

In SmartPIC the charge density is calculated on the highest (finest) level available at the particle position by trilinear interpolation. The result is subsequently restricted to all grid levels $n-1, \ldots, 0$ by the operator (5.37) giving the total charge density $\rho_n(x)$.

In accordance to the results of Section 3.2.4 the right hand side should include a term

$$en_0 \left[ e^{\Phi(r)/kBT_i} - e^{-\Phi(r)/kBT_i} \right]$$

with the requirement to possess a reference point of known potential, temperature, and densities. Such a point has already been used for calculation of the plasma potential: the emitter exit point.

However physics are not as simple. As shown in Section 4.5.2 the Debye length in the vicinity of the solar array where this special source term would apply ranges up to 1 m. Density in this region varies from $10^8 - 10^{12}\text{m}^{-3}$ and is distributed inhomogeneously. Since potentials from the solar array propagate into the plasma, and cause breaking of the quasineutrality condition, the method to use the Boltzmann relation with a reference point is inaccurate. Hence it is better to rely just on the net charge densities and recalculate those by including the relevant plasma physics as discussed in Section 4.5. Charge densities on the other hand are only available for the advanced fluid model.

A compromise seems to be the method to superimpose a solution based on the Boltzmann
relation by the static solution obtained by the multigrid solver with vanishing source term. This is not the most accurate method but does not require iterative solution of $\Phi$, $n_e$, and $T_e$ and thus saves computational time. When fully applying the advanced electron fluid model this problem will not be existent any more.

5.3.5 Adaptation of the Multigrid Method

Despite the fact that the multigrid method presented in chapter 5.1.4 is used in many applications it does not seem to be very stable under configurations where the fine grids are not defined throughout the computational domain, as in SmartPIC. The boundary regions, especially edges and corners, show difficulties when restricting the residual to the next coarser level. The problem is because a residual originated on level $n$ interpolated to level $n - 1$ can only be defined on the coarse level where the fine level values are available too. At the boundaries of the fine grid zone the pre- or postsmoothing operations are influenced by the sharp cut from the actual residual at level $n$ to 0 in regions where no levels $> n - 1$ are defined. Different approaches have been tried in order to cope this problem but none proved to be entirely stable.

The final approach which has proven to be unconditionally stable does not meet the principle of FMG. Much more it is an advanced smoothing method taking advantage of low frequency propagation on coarse grid levels. The method works as follows

- Starting at the coarsest level 0 the poisson equation (5.14) is iterated $N_{SIT}$ times with an initial guess of $u_{ijk} = 0 \forall i, j, k$. The value of $N_{SIT}$ has to be determined by trial and error. There is no need for perfect convergence at this point. A good enough solution is sufficient.
- The rough solution is interpolated to level 1 (5.26)
- Instead of performing prerelaxation, (5.14) is iterated again $N_{SIT}$ times.
- The new solution $u_{ijk}^1$ is interpolated again. The procedure continues until the finest level is reached
- Starting at the finest grid solution $u_{ijk}^M$ coarsification by the $R$-operator given in Section 5.3.3 is done to obtain an updated $u_{ijk}^{M-1}$. Again the solution is iterated $N_{SIT}$ in order to adapt to the corrections on level $M$.
- The procedure of coarsification and Gauss-Seidel iteration is continued until level 0 is reached and the whole cycle starts again with an updated initial solution.

This simplified multigrid method does not use any residuals or errors. It just relaxes on all levels and takes advantage of the interpolation and restriction operators. Tests have shown that the algorithm gives good results in a very short time. However it does not converge entirely due to the inherent problem that comes from coarsification (see Section 5.3.4). Details will be presented in the next section 5.4.

5.4 Numerical Verification of the Multigrid Solver

The intention of this chapter is to show the correctness of the implementation.
5.4.1 Test Objects

For verification purposes the whole computational domain was defined as free space. At one characteristic point \( p_t \) above the not existing spacecraft with coordinates \((x, y, z) = (0, 0, 1.1m)\) a test object which could either contain a specific charge or a defined potential was placed. Thus the propagation of the potential throughout the domain could be studied without disturbances caused by potentials of spacecraft parts or boundaries. First a test charge of \( q_t = 10^9 e = -1.602177 \times 10^{-19} \) C was implemented. Theoretically the potential should be radially symmetrically, given by

\[
    u(|r|) = \frac{1}{4\pi\varepsilon_0} \frac{q_t}{|r|} \tag{5.39}
\]

Since the Coulomb law is formulated for infinitesimally small charge volumina, point charges, there is some inaccurnateness for distances \(|r| \to 0\) when treating charge densities instead of point charges. In addition for \( r = 0 \) the potential is singular. Numerically the Gauss-Seidel scheme which is used by the multigrid method to smooth the solutions for the potential shows up a weak point here. The values are limited to the computational variable range so the physically correct potential can not be reproduced at this point. However another effect has a much greater impact; values that high will never be reached because they are simply smoothed away. The error for the source point is tending to infinity but is reduced at each Gauss-Seidel iteration. At the same time the potential for the surrounding points is rised erroneously. This causes a higher steepness of the potential around and a cutoff at the center point.

In the far field the propagation of the potential is limited by the number \( n \) of iterations that are computed. Theoretically the exact distribution function should be reached for \( n \to \infty \). For limited domain sizes convergence is reached very fast. The multigrid approach helps to speed up the propagation even for huge domains. However in practice there are some errors left.

5.4.2 Results

Best results with standard FMG method

This section presents the most stable results obtained with an implementation of the multigrid method described in Section 5.1.4.

The potential distribution along three lines \( c_1, c_2, c_3 \) (Figure 5.10(a)) has been printed and compared with the theoretical prediction. The simulation appears to match the real potential good at distances of 3 cm to 40 cm. In the far field the computed results converge faster to 0 but the error is in general small around 1.5–2 V. For small distances \( r \to 0 \) the error rises dramatically as mentioned above. The value at the source point, not depicted in the diagrams, reaches a value of \(-373.66 V\) for the following settings:

The above values have been approved to be optimal. It should be mentioned that for higher iteration numbers \( N_{SIT} \) and more cycles \( N_{CYCLE} \) errors in the vicinity of corners rise dramatically. \( N_{SIT} \) leads to convergence for values \( > 35 \). However the curve becomes smoother in regions of grid level boundaries if more iterations are applied.

The number of prerelaxations \( N_{PRE} \) seems to be quite high in comparison with \( N_{POST} \). This is necessary due to the adapted grid structure used for the simulation. Recalling Section 5.1.4 and 5.3.5 grid levels are not spread throughout the whole computational domain but are limited to regions of interest. This brings the following problem:

When restricting from a fine grid \( M \) to the next coarser one then \( R_{M-1}^{R_M} \) is available...
only in regions where the fine grid exists. All other points on level $M - 1$ are assigned a residual of 0. When the error is computed based on this residual the values at the boarders of the fine grid region are cut down which results in discontinuities in error and potential. To avoid this problem the number of prerelaxations is set very high which leads to the error propagating far into the regions where the fine grid is not defined. Thus the solution remains smooth at the boarders.

$N_{CYCLE}$ affects mainly the far field region where higher numbers lead to a better fitting of simulation and theoretical prediction. Unfortunately this also increases the error for small distances due to the higher number of iterations that propagate the error around the source as mentioned in chapter 5.4.1. Thus only one $V$-cycle is computed per level. Finally the number of levels is predefined by the grid generation and can only be changed with some programmatical effort.

In conclusion the multigrid method leads to quite short run times but shows up errors in the near field when calculating point sources. The modified grid with overlapping levels induces errors at grid level boundaries which can nearly be eliminated. Detailed errors can be viewed in Figures 5.10(b)-5.10(d).

**Results of the Final Version**

The experimentally developed simplified multigrid solver technique introduced in Section 5.3.5 proved to be stable and accurate. For verification the same method utilizing a test charge and printing the potential along three lines (see Figure 5.10(a)) has been used. Convergence in dependance of the number of cycles $N_{CYCLE}$ is depicted in Figure 5.11. Indeed increasing the cycle number leads to rapid convergence for even small values. For $N_{CYCLE} \rightarrow 5$ the potential converges constant against the theoretical curve. Above this value a rise in the far field distribution can be observed. This can be argued by domain boundary effects. Since at the borders of each domain the fields are bound to the Dirichlet condition $E^n = 0$ for the current level $n$ the potential is mirrored. Thus one has to assure that the distances to walls are great enough not to spoil the solution.

The influence of the number of iterations $N_{SIT}$ can be seen in Figure 5.12. All runs for this comparison have been computed for a low cycle number of 2. For only two iterations per level the potential shows steps at the boundaries of grid domains due to a lack in propagation. Convergence depends less on the iteration number than on $N_{CYCLE}$. Unfortunately at this point a common effect of all grid-based calculations affects the results. Since the Coulomb law is valid only for point charges, and one deals with charge densities which are to be constant over a region of at least one grid cell, the potential distributions in the near field appear smeared and show smoother slopes than the prediction. The effect can be observed very good in Figure 5.12. For greater $N_{SIT}$ the potential in the knee of the curve is higher than the reference. In the far field the curve converges for values around 8. For higher values the mirroring effect again plays a role and raises the far field potential.
Figure 5.10: Best results achieved with the classical FMG technique. a) Geometry of the 3 lines $c_n$ for which the potential is printed for b) Potential distribution in spatial directions $Z$, $Y$ and with ($\Theta, \varphi$) = ($\pi/4$, $\pi/4$) c) Potential distribution for line $c_1$. The error bars depict the difference of simulation and theory. d) Potential distribution in spatial directions $Z$, $Y$ and with ($\Theta, \varphi$) = ($\pi/4$, $\pi/4$)
Conclusion

The standard FMG method shows tremendous instabilities in the vicinity of domain corners and edges, and thus, is not applicable for the kind of grid utilized. Despite these heavy limitations it converges well for regions with all grid levels being defined. A modified version of the solver without the error correction scheme represents a stable alternative. Fitting to the analytical prediction is good at all distances but depends very sensible on initial parameters. Total convergence has not been achieved due to the error introduced by coarsification (see Section 5.3.4). The best configuration found was $N_{CYCL} = 6$ and $N_{SIT} = 2$. These settings result in very low errors and provide good fitting at all distances.
Chapter 6

Results

6.1 Computational Aspects

6.1.1 Grid Generation

Adaption of the grid to the solar array has shown to be more sophisticated in practice than initially thought. The main problem occurred in the fine grid domains ranging out of coarser domains in the inner corners of the step-distribution (see Section 5.2.2). Fine-tuning of the \textit{Tolerance} parameter as well as individual offsets in \(x\) and \(z\) direction led to a stable but specialized algorithm depending sensitively on the geometric parameters. However grid generation succeeded in tests for steps of 5° from 0° to 180° rotation of the solar array. Some configurations still show partial coincidence of domain boundaries on two different levels. This is mainly the case at the backside of the panels where no fine structures or fields are to be resolved. So the error induced by these faults is negligible. Figures B.4 – B.9 in the Appendix show the results for these tests in steps of 45°.

6.1.2 Multigrid Solver

In the current investigation without applying the advanced electron fluid model the multigrid solver is utilized to calculate static potentials. Those are caused by structural elements – in other words the satellite. Since the spacecraft floating potential is updated continuously this is only a semi-static solution. When comparing representative time scales for ion movement \(t_i\) and changes in the floating potential \(t_{fp}\) one receives a ratio of 1 : 2000 so in fact on an ion timescale the spacecraft potential is constant. Figure 6.1 shows an exemplary potential distribution for \(\eta_{sh} = 70\%\), \(\eta_{sh,IC} = 20\%\) and initial spacecraft potentials. It is noteworthy that at the outer domain boundaries only little mirroring effects appear. This is an additional proof for the settings for the multigrid solver are well chosen.

![Exemplary potential distribution](image)

\textbf{Figure 6.1:} Exemplary potential distribution around the solar array for \(\alpha = 0°\)
6.2 Verification with Ground Measurements

As for previous versions of SmartPic the plasma flow parameters have been verified with the help of vacuum chamber ground tests [32]. Such have been performed in the framework of an ESA/Estec project for characterization of electric diagnostic packages applied on recent satellites with electric propulsion systems. The measurements have been conducted in the PIVOINE facility of Aerothermique Laboratory operated by LABEN Proel based in Orleans-France. Results are not published but available in form of a report, subject to copyright and property limitations [41]. Originally these experiments were part of a ground test campaign for the French Stentor satellite that was lost in the 2002 Ariane-5 launch failure. Hence all tests mentioned in the report by LABEN have been conducted with a SPT-100 Hall thruster. Since the main characteristics of the SPT-100 and the PPT-1350 thrusters are very similar it was found to be representative to simulate conditions for the latter one by operating a SPT-100 at 350 V discharge voltage.

6.2.1 Experimental Conditions

The electric plasma diagnostic packages utilized consist each of one retarding potential analyzer (RPA) and one Langmuir probe (LP). Both sensors are mounted in one common housing with an extension arm.

The RPA is a flat gridded wide aperture analyzer, made of a ceramic body containing a stack of 4 metallic grids standing over a metallic target which collects the ions. Geometrically the construction is cylindrical with 46 mm diameter and 30 mm aperture length. A circular, planar LP of 2 mm diameter specially designed for the expected vacuum test conditions is mounted on an extension arm attached at the housing.

Sensor packages have been distributed at different angles to the beam axis and varying distances from the exit. 4 test scenarios have been run, each simulating different conditions and requiring unique configurations for the RPA geometry. Two of these scenarios are of interest for validation of the PPT-1350 conditions on SMART-1. The first one includes measurements at low beam angles, the second one is an investigation of the CEX environment at high angles. The geometry of the SMART–1 EPDP RPA could not be set up due to limitations in the vacuum chamber.

Coordinates of the RPAs used in the simulation are found in Table 6.1. General parameters of the LABEN tests and the according set for computation is given in Table 6.2.

<table>
<thead>
<tr>
<th>Ref. No.</th>
<th>d [mm]</th>
<th>α [°]</th>
<th>β [°]</th>
<th>Ref. No.</th>
<th>d [mm]</th>
<th>α [°]</th>
<th>β [°]</th>
</tr>
</thead>
<tbody>
<tr>
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<td>670</td>
<td>-10.0</td>
<td>0.0</td>
<td>7</td>
<td>1,092</td>
<td>21.5</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>670</td>
<td>0.0</td>
<td>0.0</td>
<td>8</td>
<td>1,035</td>
<td>11.2</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
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<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>670</td>
<td>10.0</td>
<td>0.0</td>
<td>10</td>
<td>800</td>
<td>60.0</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>670</td>
<td>15.0</td>
<td>0.0</td>
<td>11</td>
<td>215</td>
<td>88.0</td>
<td>61.0</td>
</tr>
<tr>
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<td>670</td>
<td>20.0</td>
<td>0.0</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 6.1: Geometrical positions of RPA sensors taken for comparison with simulation.
Figure 6.2: Geometry of RPA positions. Coordinates are given by the distance to the thruster exit \(d\), the angle \(\alpha\) of the RPAs line of sight to the thruster exit relative to the beam axis \(z\). Additionally an angle \(\beta\) between the line of sight and the RPAs normal axis is given. Ions enter the RPA at the incidence angle \(\gamma\).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Exp.</th>
<th>Sim.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>bar</td>
<td>2.7-3.2(2.83)×10^{-8}</td>
<td>2.83×10^{-8}</td>
</tr>
<tr>
<td>Neutral temperature</td>
<td>K</td>
<td>–</td>
<td>300</td>
</tr>
<tr>
<td>Electron temperature</td>
<td>eV</td>
<td>7.75-8.53(0.803)</td>
<td>0.832</td>
</tr>
<tr>
<td>Ion temp. axial</td>
<td>eV</td>
<td>–</td>
<td>1.7</td>
</tr>
<tr>
<td>Ion temp. radial</td>
<td>eV</td>
<td>–</td>
<td>0.4</td>
</tr>
<tr>
<td>Acceleration voltage</td>
<td>V</td>
<td>350-15</td>
<td>335</td>
</tr>
<tr>
<td>Mass flow anode</td>
<td>mg/s</td>
<td>3.95-5.34 (4.99)</td>
<td>4.63</td>
</tr>
<tr>
<td>Mass flow cathode</td>
<td>mg/s</td>
<td>0.44</td>
<td>0.40</td>
</tr>
<tr>
<td>Discharge current</td>
<td>A</td>
<td>4.28</td>
<td>–</td>
</tr>
<tr>
<td>Spacecraft potential</td>
<td>V</td>
<td>Ground (biased)</td>
<td>0</td>
</tr>
<tr>
<td>Potential anode</td>
<td>V</td>
<td>335</td>
<td>335</td>
</tr>
<tr>
<td>Potential cathode</td>
<td>V</td>
<td>-15</td>
<td>–</td>
</tr>
<tr>
<td>Potential at exit</td>
<td>V</td>
<td>–</td>
<td>15</td>
</tr>
<tr>
<td>Spatial Domain</td>
<td>m^3</td>
<td>Vac. chamber 2×3×2.8</td>
<td>9×10^9</td>
</tr>
</tbody>
</table>

Table 6.2: Physical parameters of the experiment compared with Simulation inputs. Remark: ‘–’ depicts an unknown or not applicable value.

6.2.2 Results and Discussion

Low Angle Measurements

Data from low angle RPA positions (|\(\alpha| < 45^\circ\), Ref. No 1-9) represent plasma data in the main beam. Detected ions show an approximate Maxwellian velocity distribution around the initial energy equivalent to the acceleration voltage of the thruster. Energy loss due to potential gradients and collisions in the beam cause broadening and shifting of the primary peak. Results for the energy peaks fit well within the given standard deviations of \(\pm 18\) eV (see Figure 6.3(a)). Generally simulation results show higher peak energies than the experimental data. This can be explained by the initial ion velocity distribution used for simulation which in fact is constant at the initial velocity \(v_i\) according to the acceleration voltage (see Section 4.1) with a Maxwellian add-on. Since \(v_i\) represents the maximum velocity possible for a distinct discharge voltage the mean velocity peak is shifted...
to higher energies compared to the experiment. LABEN reports that a drop in ion energy by the order of the plasma potential of $\approx 25\,\text{V}$ can be expected. This is physically reasoned by the ions running up a potential hump on the beam axis close above the thruster exit. This hump, typical for Hall thrusters, is observed to be smaller in the simulation ($\approx 12 - 18\,\text{V}$). This again gives rise to a positive difference in the results.

![Comparison of the RPA peak energies and FWHM values for simulation and experiment at different angles ("angle sweep") relative to the beam axis.](image)

**Figure 6.3:** Comparison of the RPA peak energies and FWHM values for simulation and experiment at different angles ("angle sweep") relative to the beam axis.

However, ion energy distribution functions of experiment and simulation fit within the peak value offset of $25\,\text{eV}$ shown in Figure 6.3(a). Error bars depict a constant standard
deviation of ±18 eV taken from [41].

Regarding the width of the primary RPA peaks the constant velocity distribution used in the simulation causes small values for the full width at half maximum (FWHM). Here again experimental results are influenced opposite to the simulation. The disturbance due to the vacuum chamber walls has not been taken into account in the computer calculations. Walls reinject scattered ions into the beam and increase collisional effects.

According to LABEN the PPS-1350 condition is characterized by high fluctuations in ion energy resulting in additional spreading of the energy peaks. These two facts explain the difference observed in Figure 6.3(b).

Nonetheless it is remarkably that despite of the tight initial band for ion velocities the FWHM values obtained by simulation do not vanish. The broadening is reasoned by the Maxwellian add-on to the velocity distribution and locally fluctuating electric potentials in the beam.

Measurements at higher distances (around 1 m) show a slight decrease in peak values compared to the results of the 670 mm tests. Again, as concluded in [32], the simulation is more accurate than the experiment at this point. Computed results for $\alpha = 0^\circ$ match for 670 mm and 1,016 mm (Figure 6.4(a)) while experimental data shows a significant decrease in peak energy. The measured RPA curve does not agree with the peak value of 332 eV given in the angle sweep test (vertical blue line in Figure 6.4(a)). This has not been explained by LABEN and is most likely due to an offset error in the experiment since at positions very close to $0^\circ$ no such shift can be seen.

In SmartPIC data (Figures 6.4(a) – 6.4(c)) one observes that peaks for the 1 m locations are shifted to lower energies by $2 - 7$ eV. The effect is most prominent for the $0^\circ$ samples. This can be explained by the electric potential hump which is situated in the beam center, and creates a downhill run for ions from the point of highest density at $\approx 20$ cm above the thruster exit to the outer plume regions. In the center line of the beam the potential decreases much less. Hence ions at $\alpha = 0^\circ$ cannot acquire much energy. The downshift in general, for the experiment, can be explained by low-angle collisions in the beam. For the simulation the most likely cause are the fluctuations due to a coarse PPP ratio (see Section 6.4.1) leading to a similar effect as low angle scattering. This is a point requiring further investigation.

In conclusion the agreement between experimental data, and simulated data by SmartPIC is very good for RPA positions in the beam of the SPT-100 Hall thruster. Full widths at half maximum are low in the simulation due to a simplification of the thruster model. Peak energies are predicted well within the given error ranges of the measurements.

Remark: For data smoothing in some graphs a so called Fast Fourier Transformation Smoothing (FFT) method has been utilized. It filters components of the data with wavelength shorter than the interval defined by a discrete number of data points (pt). This is very useful to eliminate noise.
Figure 6.4: Comparison of RPAs at distances around 1 m within the beam. Stentor data is always confronted with SmartPIC output at 670 mm and the appropriate data for 1 m. Positions are defined in Table 6.1
High Angle Measurements

Data from high angles (\(\alpha > 45^\circ\)) represent CEX plasma data. Ions reaching RPA 10 have been scattered out of the beam by collisions. So comparison of numerical data to experimental results for this position provides information on the validity of the collision model and correctness of the electric potential distribution causing transport of the particles. In the LABEN tests the EPDP position on SMART–1 could not be set up due to geometrical restrictions of the vacuum chamber. So the only high angle measurements available are those of RPA 10 and 11.

Common to all data sets is the dominant CEX peak below 20 eV. Above this level only diffuse scattered intensity below 10% of the peak value is seen. Solely RPA 10 which is just 13° out of the beam shows a little hump of beam ions at \(\approx 318\) eV. These could be the result of very low angle scattering with neutrals at the thruster exit. [32] explain the occurrence of high energetic ions at this angle by just higher nominal thruster divergence. In fact the hump is below 10% of the CEX peak at this position and below 1% of the peak at 0°.

The current SmartPIC version shows good agreement with the experimental results. The CEX peak is met exactly in width. Stray intensity levels in the energy domain 20–200 eV agree. A little deviation can be seen in the energy of the primary ion peak which is \(\approx 2\) eV too high in the simulation.

Figure 6.5: Comparison of wide angle data for RPA 10. Note that simulation data have been shifted by \(-25\) eV conformal to the offset given by [41].
6.2.3 Conclusion

Virtual RPAs at 11 different positions have been implemented to compare experimental data with simulation results. In general there is good agreement. Analysis at distances of 670 mm within the main beam at low angle shows no significant variations of peak energies with the position. SmartPIC predicts sharper peaks in velocity distributions than measured by LABEN due to a simplified thruster model. Analysis for small angles at higher distances confirms the simulated results obtained at 670 mm. Over all SmartPIC data show very good agreement with the measurements in the low angle domain. High angle RPA data is representative for the CEX environment. SmartPIC predicts the primary peak at energies below 20 eV as well as the secondary peak with high precision. This can be seen as a verification of the potential solution throughout the beam and the collision model.

6.3 Verification with SMART-1 Data

6.3.1 Conditions

The single RPA of the EPDP (see Section 2.3.1, Figure 2.6) has a very extreme position of \( d = 570 \) mm, and \( \alpha = 85^\circ \) relative to the thruster exit. Hence the data obtained with EPDP is representative for CEX backflow. Unfortunately there is no information available about the actual tilting angle \( \beta \). According to [42], and internal ESA reports, the SMART–1 RPA curve has to be shifted by \(-11\) to \(-18.5\) V (see also Section 2.3.1).

6.3.2 Results and Discussion

SmartPIC results agree very well in the peak energy, and FWHM with the measurements. The peak at 20.8 eV is 1.3 eV below the maximum shift boundary. This is acceptable if one considers deviations of \( \pm 1 \) eV for different simulation runs. Moreover the \(-18.5\) eV shift announced by ESA seems to be too low if, for example, considering the shift in Figure 2.8(b) which is approximately 20 eV. Unfortunately there is no information about the exact tilting angle of the EPDP RPA available. Figure 2.6 which is provided by ESA shows an approximate tilting of 20°. In order to find the correct setting the expected RPA response has been calculated for several values for \( \beta \) listed in Table 6.3. As can be seen from Figure 6.6 both, peak energy, and FWHM decrease monotonically with rising tilting angle. Hence there is definitely one single solution for a best fit with the measurement data. This is at \( \beta = 20^\circ \).

<table>
<thead>
<tr>
<th>(\beta [^\circ])</th>
<th>(E_{max} [\text{eV}])</th>
<th>(FWHM [\text{eV}])</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>21.0</td>
<td>17.0</td>
</tr>
<tr>
<td>10</td>
<td>21.0</td>
<td>16.7</td>
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<tr>
<td>15</td>
<td>20.8</td>
<td>16.3</td>
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<td>20</td>
<td>20.4</td>
<td>15.2</td>
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<tr>
<td>30</td>
<td>18.8</td>
<td>10.2</td>
</tr>
<tr>
<td>67</td>
<td>5.0</td>
<td>3.5</td>
</tr>
</tbody>
</table>

Table 6.3: SmartPIC results of RPA responses of the SMART–1 EPDP RPA for different tilting angles \( \beta \). Peak energy \( E_{max} \), and FWHM both fall with increased \( \beta \).
Regarding the absolute values of the relative intensity no direct comparison of SmartPIC data with in-flight data can be given. In fact the absolute values of dI/dE are higher by a factor 3-5 compared to all experimental results presented in this work. Hence only normalized comparisons are given. The values in Figure 6.6 refer to the measurement. Simulation data have been normalized to $2.5 \times 10^{-7}$ eV/A. A reason for the scaling is currently under investigation. The most likely cause is an error in the CEX generation for collisions.

**Figure 6.6:** Dependence of the peak energy and FHWM of SmartPIC results on the tilting angle $\beta$

Remarkably good agreement between measurement and simulation have been obtained with regard to the prediction of the secondary peak. According to [43] the secondary peak is due to single charged Xe$^+$ products of the reaction Xe$^{2+}$ + Xe$^+$ $\rightarrow$ Xe$^+$ + Xe$^{3+}$

**Figure 6.7:** Comparison of flight-data from SMART-1 EPDP with SmartPIC data. The upper and lower boundary curves resulting from the unknown offset are depicted in grey.
which is indeed included in SmartPIC, and should appear at twice the energy of the main peak. Figure 6.7 shows a secondary peak in simulation data at approximately 37 eV which is 4.8 eV below the expected position. However since in-flight data shows even greater deviations from the 1:2 ratio of primary, and secondary peak this may indicate that the maximum shift had to be set to 22.5 V instead of 18.5 V.

6.4 Flow Analysis

6.4.1 Influence of the Particle Ratio

The ratio of computer particles per real particle (PPP) defines the resolution of density distributions. Several physical variables directly depend on densities. Too high PPP ratios cause unphysical fluctuations and hence high E fields that further lead to diffuse scattering of CEX ions. So it is advisable to use low ratios.

On the other hand some parts of the program exhibit an \( O(N^3) \) behavior in the total number of computer particles \( N \). In fact it is a trade-off between accuracy and run times. The final version excluding the new electron model takes approximately 2 days for 1.2 ms at \( PPP_i = 5.0 \times 10^9 \), \( PPP_n = 1.0 \times 10^{10} \), and \( PPP_{CEX} = 2.0 \times 10^8 \) which shall be referred to as scenario 1. Increasing fineness to \( PPP_i = 1.0 \times 10^8 \), \( PPP_n = 1.0 \times 10^{10} \), and \( PPP_{CEX} = 1.0 \times 10^8 \) (scenario 2) results in 2 days for 50 \( \mu s \).

![Figure 6.8: Comparison of the ion density flow field near the thruster exit for scenario 1 on the left, and scenario 2 on the right. It has to be mentioned that the CEX flow outside the beam is not fully formed on the right since the simulation took 3 days for only 75 \( \mu s \) while for the left side an output at 700 \( \mu s \) has been taken. Black lines depict domain level boundaries. Unit: [m\(^{-3}\)]](image-url)

Regarding the physical correctness a direct comparison for the main beam flow field has been set up. The PPP parameters correspond to those of scenario 1, and 2. Results are depicted in Figure 6.8. For the high PPP ratio the flow field shows some holes in the domain of highest spatial resolution. As discussed in Section 4.5.2 at the highest density close to the thruster exit there are at average only 7 computational particles in one grid
cell. In regions of density $10^{14}\, \text{m}^{-3}$ the same calculation results in 0.013 particles per cell which explains the holes. For scenario 2 no such breaches can be seen. For $10^{14}\, \text{m}^{-3}$ the PPP ratio of $1.0 \times 10^8$ results in 0.6 particles per cell. This is not quite much too but sufficient to provide a smooth density distribution. The resulting electric fields depicted in Figure 6.9 agree with these thoughts.

![Figure 6.9: Comparison of the electric field in Z direction near the thruster exit for scenario 1 on the left, and scenario 2 on the right. High field amplitudes and fluctuations appear in regions of high spatial resolution above the thruster exit for the coarse PPP ratio. For scenario 2 the field configuration is smooth and regular. Unit: [Vm$^{-1}$]](image)

### 6.4.2 CEX Flow to the Solar Array

For the analysis of the CEX backflow to the solar array the current density is monitored on the front and back sides of the solar array independently. The results are depicted in Figures 6.10 – 6.14. Coordinates are given in units of $[\Delta x_5]$ with the origin at the (+X,-Y) corner of the solar array. Plots for front side and back side are both oriented parallel. This means that the views equal those obtained when looking at the array from the solar cell side. For this investigation the spacecraft potential was not updated. Shielding was set to $\eta_{sh} = 70\%$, and $\eta_{sh,IC} = 20\%$. The plots represent integrated data $0 - 1.28\, \text{ms}$.

The main ion collectors on the front side are obviously the metallic structure parts between the interconnectors since they are biased to spacecraft ground. Additionally the edges of the spacings between the panels face the CEX plasma flow, and hence act like “ram” surfaces nearly independent of the actual angle. For low rotation angles $\alpha < 45^\circ$ only a few computer particles are able to reach the back side of the array. It is likely that the particles follow the field lines of the potential emerging the front side (see Figure 6.1). For higher angles $\alpha \to 90^\circ$ one can observe a clear gradient from $+Z$ (top) to the lower regions on the back while the distribution on the front side is still relatively homogeneous with only a slight gradient. High densities can be seen at the $+Z$, and $-Y$ edges of the
array. At $\alpha = 135^\circ$ the current to the front side nearly vanishes. This agrees very well with the results in Section 6.5.1. For the backside with its attractive potential for ions a uniform, radial decreasing current distribution can be seen at $\alpha = 180^\circ$.

![Figure 6.10: Ion backflow to the solar array at 0°](image)

![Figure 6.11: Ion backflow to the solar array at 45°](image)
Figure 6.12: Ion backflow to the solar array at 90°

Figure 6.13: Ion backflow to the solar array at 135°
Figure 6.14: Ion backflow to the solar array at 180°

Figure 6.15: Legend for Figures 6.10 – 6.14. Current densities in [Am^{-2}].

The calculation of backflow current distributions provides an essential input for future solar array design. In order to reduce spacecraft floating potentials it will be necessary to minimize collective surfaces. This assessment has shown that bare metallic structures in the vicinity of electric fields are the main ion current collectors. Hence alternative geometries have to be found exhibiting a minimum of conductive surfaces at potentials different to spacecraft ground. This topic will be discussed more detailed subsequently in the next sections.
6.4.3 Densities

In order to understand the effects which cause spacecraft charging it is important to get information on the 3-dimensional flow of the particles. This analysis gives information on how ion trajectories are influenced by the spacecraft potentials.

For all outputs depicted in this section the PPP settings referred to as “scenario 1” in Section 6.4.1 have been utilized. Shielding factors were $\eta_{sh} = 70\%$ and $\eta_{sh,IC} = 20\%$. The spacecraft ground was not updated for this investigation.

**Main Beam**

The exhaust beam above the thruster exit is formed mainly by neutrals and primary beam ions. The highest densities can be seen at the exit of the thruster cavity and at the interference point of the inner beam boundaries approximately 10 cm above the thruster exit.

Since kinetic energies of beam ions are above 300 eV these particles cannot be redirected significantly by the electric fields. Only CEX ions with initial energies of below 1 eV are influenced by the radial electric potential gradient created by the plasma column of the beam.

Figures 6.16(a) – 6.16(d) show a XZ-slice of the region above the thruster exit. The relevant legend for densities is included in Figure 6.16(a); unit: [m$^{-3}$]. From the difference
of Figures 6.16(a) which depicts the total ion density, and 6.16(b) which shows CEX ions only, one can observe that beam ions indeed stay within the beam cone while the low energy particles expand in all directions. Double charged CEX ion (DCCEX) account for approximately 8% of the total flow. Accordingly the densities in 6.16(c) are lower. Generally one can observe a slight asymmetry in the flow field in the vicinity of the thruster exit. Densities on the +X side (right) are higher than on the opposite side of the beam. This can be explained by the position of the negatively biased neutralizer at \((x, y, z) = (85\, mm, 15\, mm, 10\, mm)\) relative to the center of the thruster exit.

### 6.4.4 CEX Domain

As discussed above exterior to the beam only CEX ions can be expected. These follow the electric field lines radially away from the beam. While doing so they acquire a kinetic energy equal to the potential difference between the current position and the point of their creation. Hence the energy at a distance of 1 m from the beam axis reaches approximately \(10 – 30\, eV\). This is the region where the repelling potential emerging from the solar array’s front side starts to influence the plasma flow. Depending on the rotation angle of the array the CEX flow is redirected.

According to the superposition technique for the electric potential discussed in Sections 4.3.2 and 5.3.4 the total potential is composed from the free space solution depicted exemplarily in Section 6.1.2, Figure 6.1. The resulting total potential is depicted for the two extreme positions of the solar array rotation. Obviously the plasma potential is governed mainly by the plasma density. However relative changes in the region 20 – 40 cm above the solar array cannot be seen easily due to the relatively low number of levels depicted.

![Potential V](image)

**Figure 6.17:** YZ-slice of the total plasma potential above the solar array.

Ion density distributions of course do not differ much from potential distributions; although one can directly observe the influence of the repelling spacecraft potential in
Figure 6.18. For $\alpha = 0^\circ$ only a few ions make the way through the potential barrier of the array. A line of reflection ascending from left to right can be observed. With the solar array turned by $180^\circ$ no such effect can be seen. This correlates with the results in Section 6.4.2. For $\alpha = 90^\circ$ the density is depicted in the XY plane on the height of the thruster exit. A clear asymmetry can be observed. Again the repelling effect of the solar array governs the flow.

Finally the displacement of ions at the $+Y$ plane of the main body can be observed by comparing magnified views of the density distribution above the extension arm. Results are depicted in Figures 6.19(a), and 6.19(b). The solar array tilted by $90^\circ$ clearly reduces the ion flow in between the array and the main body.

Figure 6.18: Slices of the ion density distribution. Unit: $[m^{-3}]$
6.5 Spacecraft Floating Potentials

6.5.1 Reproduction of Previous Results

For the verification purposes of the current simulation, the output is compared to the results of previous versions already published and accepted [35]. In order to produce comparable data, the input parameters for both versions are identical. Updating of the spacecraft floating potential has been disabled for these tests. In fact the only differences in the physical model remaining are

- shielding solely for glass covered parts of the solar array. In previous versions all surfaces on the panels, including interconnectors, have been shielded
- multigrid environment with partially higher spatial resolution
- periodical update of free space potentials and plasma potentials
- slightly changed spacecraft geometry corresponding to real structure dimensions

Results

In comparing and validating the current version a confrontation of the most important parameters affecting the calculation of floating potentials has been conducted. The results are depicted in Figures 6.20 – 6.21.

Discussion

Principally the current results match those published in [35] qualitatively. In fact there are some differences due to effects that will be discussed subsequently.

Ion currents depicted in Figure 6.20(a) show agreement of the two versions within a factor 2. In comparison to previous results ion currents to the main body are reduced for a vertical position of the solar array. This can be reasoned by the high positive potentials emerging from the unshielded interconnectors displacing ions from the Y-planes of the main body. In general the backflow to the spacecraft main body is roughly independent of the solar array rotation. Ion currents to the solar array monotonously rise for $\alpha = 0^\circ \rightarrow 180^\circ$. This is due to the positive potentials on the front side of the array repelling ions while the back side is biased to spacecraft ground, which is negative with
Figure 6.20: Comparison of the most important parameters for floating potential calculation. a) depicts ion currents on different parts of the spacecraft. b) compares the mean surface areas collecting electrons. c) shows the calculated electron currents based on Equation (4.15). Abbreviations prev. for previous version, and curr. for current version results.
Figure 6.21: Comparison of the floating potential achieved with previous and current versions of SmartPIC, and flight data from June, and November 2004.

respect to the plasma, and attracts ions. Currents to the extension arm are roughly constant.

Regarding the absolute amplitudes, the spacecraft main body represents the main ion current drain for the plasma with a total of $5 \times 30$ mA. This is intentionally clear because the highest CEX densities are in the vicinity of the thruster as was shown by [10]. Currents to the solar arrays are lower by at least one order of magnitude ($10^{-1000} \mu A$). Due to the little surface area backflow to the extension arm plays a minor role with currents $< 10 \mu A$.

Current collecting surface areas are depicted in Figure 6.20(b). These are calculated by integrating the surface area being hit by ions for every time step. The presented values are time-averaged over 150 $\mu s$.

For the main body the effect of the ion repelling solar array potential can be seen again for $\alpha = 90^\circ$. For more horizontal positions of the arrays the influence is weaker and more ions are attracted by side panels of the main body. Generally previous results show lower ion collecting surfaces to the for this part of the spacecraft. This is reasoned by the very coarse grid resolution in the new version of $\Delta x = 137.5$ mm on the side planes of the cube. Since backflow is observed only near the upper $+Z$ edges (see Figures 6.16(a) – 6.16(c)) in previous versions with $\Delta x = 25$ mm a maximum of 0.1 m$^2$ could be expected while for the new version the same distribution results in 0.53 m$^2$.

The solar array structure (excluding interconnectors) exposes a maximum surface area for vertical positions when being closest to the beam. In contrast to previous versions backflow areas on the back side of the solar panels for positions $\alpha > 135^\circ$ are less. Interconnectors expose surface for $\alpha = 45^\circ$ when the front side still faces the beam but is not near enough to repel ions early, preventing backflow to the array.
Electron currents depicted in Figure 6.20(c) are the results of calculations according to Equation (4.15). This comparison shows great differences. Most obvious electron backflow currents to the main body, and solar array are of the same order as the electron current to the interconnectors. In previous calculations these currents were lower by several orders in magnitude. For the solar array structure this can be reasoned due to the newly introduced metallic structure parts between interconnectors (see Figure 2.5). These structures receive relatively high currents due to the proximity to the positive potentials of the interconnectors. Hence the solar array electron backflow has to be higher compared to that in previous versions. Accordingly the trend in dependence on the rotation angle is the same as for the interconnectors. The latter ones draw the main electron current which is due to the exponential proportionality on the surface potential in Equation (4.15). Despite not being shielded and hence exhibiting higher potentials, the interconnectors draw less current compared with previous SmartPIC versions. The most likely explanation is the reduction in effective collecting surface area. In fact, as can be seen in Figure 6.20(b), the collecting areas are lower by a factor 10^-1,000. The total shielding of 70% in previous versions gives approximately a factor 3.3 in the potential which corresponds to an exponential factor 27 which the electron currents in the current version with unshielded interconnectors should be higher. From these estimates one can see that the attenuation of the current by the higher surface potential is compensated completely by the reduced area. This assessment is supported by the correlation between the curves for the interconnector current and area in Figures 6.20(c), and 6.20(b) respectively. The only time the ratio of interconnector areas of previous versions and the current version falls below 100 (at $\alpha = 45^\circ$) corresponds to the only point where electron currents in the current version exceed the comparative value of previous versions. In contrast to that it is unclear why the interconnector current drops at $\alpha = 90^\circ$ while the the current to the solar array which should be correlated to the interconnector current according to the preceding considerations reaches a maximum. The latter fact is likely due to the solar array being closer to regions of high CEX density. Finally an explanation for the high current to the main body cannot be found easily. Most likely this is due to high plasma potentials at the +Z-plane of the main body.

The final result of this calculation is the spacecraft floating potential $\Phi_{SC}$ depicted in Figure 6.21. Qualitatively there is good agreement between current results and flight data. The potential rises slightly between 0° and 45°. A steep slope for $\alpha \approx 45^\circ \rightarrow 110^\circ$ follows. Finally for higher angles the potential remains roughly constant at a more positive level. In fact the amplitude of the floating potential variation is too high in the current version. The most likely reason arises from the unshielded interconnectors. The total electron currents of previous and current versions match roughly at $\alpha = 0^\circ$. For greater rotation angles the difference increases until it reaches a factor 3 for $\alpha = 90^\circ$ and reduces again for $\alpha \geq 135^\circ$. this explains the amplitude of $\Delta \Phi_{SC} = 30$ V compared to $\Delta \Phi_{SC} = 7$ V of previous SmartPIC versions and $\Delta \Phi_{SC} = 8 - 14$ V of SMART-1 data. Tests with little shielding of $\eta_{sh} = 20\%$ for interconnectors show a clear reduction of the amplitude which can be seen as argument for interconnector shielding in disagreement to the results of [34]. The influence of interconnector shielding will be discussed in the next section.
These results show that bare metallic surfaces biased to positive potentials relative to the spacecraft and exposed to plasma play a major role for the build-up of floating potentials. Since the collected electron current depends exponentially on the relative potential between the plasma and spacecraft surfaces the resulting differential potential scales very sensitively with bias voltages. In order to fulfill ever increasing power requirements bus voltages on recent spacecraft are raised to 100 V in comparison to 24 – 50 V used in the past. This not only increases the expected floating potentials by at least a factor exp(2) but raises effects not included in the current calculation. [34] showed that for bus voltages $U_{BUS} > 70$ V a leap in secondary electron emission can be expected. This additionally increases the electron backflow and, hence the floating potential. Ground tests [18]-[19] show that arcing is expected above approximately 300 V which could easily be reached with the mentioned increase of the bus voltage. However it has also been shown that so called “wrapthrough” interconnectors that are situated underneath the solar cells not being exposed to the surface increase the threshold voltage for sparking somewhat above 400 V. Additionally this would reduce the effective electron collecting surface by far.

In the case of the SMART–1 solar panels covering of the metallic structure parts situated between the inner interconnector lines as well as the side faces of the solar array at the ±X edges would be advisable. These surfaces have been shown to account for electron currents of the same order as the nearby interconnectors (see Figure 6.20(b) and 6.20(c)). However complete insulating the entire array is not the best solution because that would increase the susceptibility for differential charging which in fact again may result in sparking.

### 6.5.2 Influence of the Interconnectors

In order to investigate the influence of the interconnector potentials on the spacecraft floating potential a test for different rotation angles at $\eta_{sh,IC} = 20\%$ has been conducted. All parameters are the same as for the comparison in Figure 6.21, Section 6.5.1. Results are depicted in Figures 6.22 – 6.23. In fact the differences to the results obtained without interconnector shielding in Figure 6.21 are significant. The amplitude of the variation with the rotation angle $\Delta \Phi_{SC} (\alpha)$ is reduced from 30 V to 15 V which agrees very good with measurements on SMART–1. The absolute offset of approximately 4 V to flight data from November 2004, and 13 – 19 V to the data acquired in June 2004 does not represent an error since the flight data itself shows major variations over time. A comparison of runs at $\eta_{sh,IC} = 0\%$ and $\eta_{sh,IC} = 20\%$ shows the influence of interconnector shielding in detail in Figures 6.23(a) – 6.23(c).

In general the amplitudes of the variations with changing rotation angles flatten for increased interconnector shielding. This can be seen for ion currents as well as for effective collecting areas. Electron currents show a slight anomaly at $\alpha = 90^\circ$.

The ion backflow depicted in Figure 6.23(a) shows a general increase of the solar array component for non-vanishing interconnector shielding. This can be explained by a reduced repelling potential on the front side of the array, permitting more ions to reach the surface. Accordingly the collective areas of interconnectors rise while the amount of ions hitting the solar array is reduced in comparison to the run with no shielding. Collective areas of the main body are increased since ions are less repelled by potentials from the solar array, and more ions enter the region around the extension arms to the ±Y panels of the spacecraft body.

The characteristics of calculated electron currents for $\eta_{sh,IC} = 20\%$ are more likely to the results obtained in previous versions of SmartPIC (see Figure 6.20(c)). Electron backflow
Figure 6.22: Comparison of the floating potential obtained by SmartPIC at $\eta_{sh,IC} = 20\%$, and flight data from June, and November 2004.

to the interconnectors remains nearly constant while currents to the solar array, and main body show a monotonic increase with rising rotation angle. At $\alpha = 90^\circ$ currents to the main body and solar array drop by approximately two orders in magnitude. This effect is subject to current investigation. Although the absolute values of previous results, and those obtained with the current version and non-vanishing $\eta_{sh,IC}$ still differ by orders in magnitude a trend to lower electron currents for all components except for the interconnectors is observable. This can be seen as a partial convergence of current and previous versions at higher shielding $\eta_{sh,IC}$. However the available data is not sufficient to permit such general statements. A detailed investigation should be conducted.

In conclusion the results obtained by SmartPIC clearly state that metallic structures biased to positive potentials play a major role in spacecraft charging. Space charge limitation indeed is relevant for the small sized interconnectors on SMART–1. Best agreement with in-flight data could be achieved for a simulated shielding of $\eta_{sh,IC} = 20\%$. Systematic investigation by varying $\eta_{sh}$, and $\eta_{sh,IC}$ should be conducted. To further investigate the influence of shielding on the floating potential a thorough parametric investigation would be necessary.
Figure 6.23: Comparison of the most important parameters for floating potential calculation. a) depicts ion currents on different parts of the spacecraft. b) compares the mean surface areas collecting electrons. c) shows the calculated electron currents based on Equation (4.15). The values 0, and 20 refer to the percentage of interconnector shielding.
6.5.3 Results with Updated Floating Potential

Updating brings the effect of direct coupling between the amount of backflow and the spacecraft potential. Despite of being physically correct this introduces major errors due to not respecting the sheath when calculating the floating potentials. Setting the spacecraft ground to a negative potential $\Phi_{SC} = \Phi_f < 0$ V with respect to vacuum leads to increased attraction of ions and accordingly higher ion densities at the surfaces of the solar array. This further influences the calculation of the floating potential. Higher ion backflow equals higher electron currents according to Equation 4.15. This again leads to a more negative floating potential. Due to the exponential dependence on the surface potential this circle does not lead to complete instability but causes too high negative floating potentials around $-100$ V to $-120$ V. Updating of the spacecraft ground has indeed been tested with different settings for shielding, and solar array rotation angle. The result is always a much too negative potential in the range mentioned above. Since there are no better results expected due to the error being inherent to the utilized model used for the calculation of the floating potential investigation on this topic has been stopped and will be continued when the new electron fluid model is completely implemented.

6.5.4 Comment on SMART–1 Floating Potential Data

The floating potential data depicted in Figures 6.21 and 6.22 has been provided by ESA. The actual curves were obtained by applying Equation (2.3) (see Section 2.4.2) on $U_{crp}$, and synchronizing in time with the rotation angle of the solar array. The November data depicted in Figure 6.21 is limited to one orbit (November 15th – 19th, 2004) while the respective curve in Figure 6.22 represents flight data from the complete month (November 2004). Available data from June 2004 is very fragmented and incomplete. This is the reason why only data for angles $78^\circ < \alpha < 165^\circ$ are depicted. However the curve represents data of the entire month. The most important thing to observe here is that the absolute value of the spacecraft floating potential varies with time. The difference between data from June, and November totals in $12 – 15$ V. Even within one month a variation of $2 – 5$ V can be seen. The cause of these variations is principally unknown. This is the reason why the offsets of SmartPIC results relative to flight data in Figures 6.21, and 6.22 do not represent a fault. One effect worth future investigations is the temporal occurrence of maxima in the curve around $135^\circ$ (see Figure 6.22). This has already been subject to internal ESA reports. Unfortunately data is inconsistent in this point, so a clear decision if the effect is real cannot be taken. However SmartPIC data indeed shows a slight decrease of the floating potential for angles $\alpha > 135^\circ$ that leaves space for discussion on a maximum.
6.6 Conclusion

The spacecraft environment plasma simulation SmartPIC has been completely revised. Review of plasma physics for low density CEX backflow regions has shown that the Debye length which is representative for the sheath size ranges up to 1 m from the solar array into the plasma. Due to inhomogeneities in the plasma and the non-trivial geometrical configuration analytical treatment in terms of the Langmuir sheath theory is inaccurate. This motivates the development of an electron fluid model capable of self-consistent calculation of the electron density distribution including conservation of charge. Pre-work for this new model included the implementation of an adapted multigrid-solver scheme working on a 6-staged multigrid with domain-subdivisioning. In addition the exact geometry of the satellite, especially the solar array, has been modeled.

The new features have been tested and verified against analytical data and experimental results. Furthermore the ion energy measurements by the SMART–1 EPDP RPA have been reproduced. A comparison of this in-flight data against the predictions of SmartPIC showed the high accuracy of the simulation. Finally calculation of floating potentials utilizing an existing model based on the balance of backflow currents has been conducted. Results have been compared to outcomes of previous versions of SmartPIC and flight data. Principal agreement could be achieved. A cyclic variation of the spacecraft floating potential with the rotation angle of the solar array has been observed on SMART–1. This effect has been predicted by SmartPIC at high accuracy. It has been found that positively biased metallic structures play a major role in the formation of floating potentials due to increased electron attraction. Interconnectors which are located between the solar cells on top of the arrays and electrically connect solar cells at positive potentials up to 50 V are exposed to the plasma. These structures draw high electron currents, and hence cause negative charging of the spacecraft. The amount of electron backflow, varies with the effective current collecting surface, that further depends strongly on the rotation angle of the solar array. If the cell side of the panels faces the thruster exhaust plume high electron backflow currents can be observed which result in negative potentials of $-35$ V to 20 V. Turning the solar array by 180°, so that the conductive back side biased to spacecraft ground faces the plume, reduces the floating potential to approximately $-15$ V to $-5$ V.

Further research has shown that the amount of space charge building up on the dielectric surfaces of the solar cells and interconnectors is an important factor since it directly influences the effective surface potentials propagating into the plasma. A reduction of the interconnector potentials by only 20% resulted in a decrease of the amplitude in the variation of the floating potential from 30 V to 15 V.

Regarding the design of future satellites an increase of the spacecraft bus voltage from 50 V to 100 V due to high power requirements of electronic devices is expected. This would dramatically increase the spacecraft floating potentials to below $-300$ V. At such voltages short circuits and even sparking may occur, leading to destruction of sensible electronics or solar arrays. Hence grounding will be a sophisticated issue of highest importance. On solar arrays the implementation of so called “interleaved” interconnectors being situated underneath the cells could be a solution to decrease the electron backflow. In general any conducting surface biased to a voltage different than spacecraft ground shall be avoided if possible.
6.7 Future Work Recommendations

No simulation can ever be complete. It is a tradeoff between doing the necessary to fulfill requirements and ambitious perfectionism trying to model nature in all its facettes and details. However SmartPIC fulfills its requirements to a far extent. As mentioned earlier in Section 1.3 time has not been sufficient to complete the implementation of the advanced fluid model. This leaves space for further development.

6.7.1 Grid

The grid generation itself is partially hard-coded including some basic structure definitions of SMART–1. It would be preferrable to completely automize this process based solely on parameters from the input file. This would enable uncomplicated structural changes in geometry, for example if another satellite had to be calculated. Furthermore the grid didn’t prove to be optimal for some of the appearing physical problems. The multigrid solver induces errors at grid domain boundaries that lead to “ripples” in the potential solution and, thus, to changed ion trajectories. The solution would be definite overlap regions of at least 4 fine level grid cells to assure correct propagation, restriction and interpolation in these regions.

One additional issue arises from physical accuracy. The Debye length, especially near the thruster exit, is still smaller by a factor 100 compared to the finest grid size. However including a domain of even smaller grid size than 0.859 mm would dramatically increase memory requirements and computational times. One has to weight better accuracy against that. In either case the multigrid Poisson solver requires a multi-level grid which contradicts the use of structured grids or other schemes providing better adaption to the Debye length or surfaces.

6.7.2 Calculation of Floating Potentials

Calculation of floating potentials in SmartPIC is principally based on the quasineutrality assumption. Since the validity of this simplification is questionable one has to think of different ways to calculate the potential. In the literature one can find some more or less advanced approaches for determination of spacecraft floating potentials. [45] gives a review of existing models and develops theory for a routine measurement technique for determination on satellites. However at this place a different approach shall be proposed. Returning to the very rudimental physics of spacecraft charging the basic assumption common to all usual models is the conservation of currents. This, undoubtable, is a reasonable and valid basis for calculations. But conservation of currents is not the most basic principle for electric charging. It is the collection of discrete charges, causing electric potentials and, thus, react on the current. Hence the most accurate calculation of a floating potential should include the influence of collected particles (which define a backflow current).

From the theory of electromagnetic fields it is known that for a configuration of $N$ insulated conductors the following relations hold

$$Q_i = \sum_{j=1}^{N} C_{ij} \Phi_j$$  \hspace{1cm} (6.1)

where $i$ and $j$ are indices of the conductors, $\Phi_i$ depicts the electric potential, and $C_{ij}$ are the electric capacity coefficients depending solely on the geometry of the configuration.
If one adapts this picture for a satellite surrounded by plasma in fact the system can be seen as a badly insulated capacitor. The total space charge in the plasma is very low and appreciable amounts of net charge can only be observed in the sheaths near surfaces. Hence for a first approximation one can assume the spacecraft to be insulated and floating in vacuum. For such a single conductor Equation (6.1) simplifies to \( Q = C\Phi_{SC} \). The difficulty now is the determination of the exact capacity \( C \) of the spacecraft. It strongly depends on the geometry and cannot be obtained analytically. A possible solution is provided by the multigrid solver. If one assumes the spacecraft as just a vacuum filled conductive hull of equal geometry and places a known uniform charge density on the surface one is able to calculate the internal potential for which Faraday states that \( \nabla\Phi = E = 0 \). Hence the potential is constant and should equal the spacecraft floating potential for the given charge. Furthermore the result should depend linear on the total charge applied. The coefficient of this linearity is the capacity being sought. This scheme has already been implemented and results for Smart–1 in a capacity of \( 1.7368 \times 10^{-10} \) F against vacuum. Bearing in mind that the expected total current from ambient plasma obtained by Equation 3.32 for a density \( 10^8 \) m\(^{-3} \) and uniform temperature of 0.6 eV initially is of the order \( 10^{-5} \) A. Assuming a transient of 0.1 ms one obtains for the spacecraft potential \( \Phi_{SC} = -5.8 \) V. This correlates excellent with theory and measurements for floating potentials on spacecraft. Encouraged by those estimates and the outlook to obtain independent electron and ion backflow currents by application of the presented new electron fluid model this capacity calculation will be developed further.

### 6.7.3 Electron Fluid Model

This point holds the most difficult tasks for future work. The model has to be tested and verified. Instabilities have to be eliminated and algorithms optimized as far as possible. In fact this is subject of current work and will be completed soon. Hopefully the electron fluid model will lead to a physically correct and complete description of the plasma interactions with spacecraft and solar cell arrays.
Bibliography


[42] Personal correspondence with Denis Estublier, Head of the SMART–1 Electric Propulsion Team, ESA/ESTEC, September 2004


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This work has been written and typeset in \LaTeX{}.
Appendix A

Technical Drawings

This Appendix includes technical drawings of SMART-1 and the solar array. The latter one is courtesy of ESA/ESTEC.
Appendix B

Simulation Figures

Figure B.1: Grid domain distribution at $x = 0$ The grid is printed in orange, level boundaries in dark green. The spacecraft is depicted in grey.
Figure B.2: Grid domain distribution near the thruster at $x = 0$
Figure B.3: Grid domain distribution near the thruster at $y = 0$
Figure B.4: Grid domain distribution around the solar array, XZ-slice, rotation: 0° Domain boarders are printed in orange, grids are colored green (for structure coloring legend see Figure B.5).

<table>
<thead>
<tr>
<th>Structure</th>
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<tbody>
<tr>
<td>Interconnector</td>
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<tr>
<td>Glass Cover</td>
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<tr>
<td>Thruster Ceramic</td>
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<tr>
<td>Thruster Cavity</td>
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<tr>
<td>Solar Array (conducting)</td>
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<tr>
<td>Spacecraft</td>
</tr>
</tbody>
</table>

Figure B.5: Legend of structure colors for figures B.4–B.9.
Figure B.6: Grid domains: Solar array, XZ slice, 45°
Figure B.7: Grid domains: Solar array, XZ slice, 90°
Figure B.8: Grid domains: Solar array, XZ slice, 135°
Figure B.9: Grid domains: Solar array, XZ slice, 180°